Supplementary Information

New Isocoumarins from the Marine Fungus *Phaeosphaeriopsis* sp. WP-26

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S1. **The ITS gene sequences data of *Phaeosphaeriopsis* sp. WP-26**

CCTGCGGAAGGATCATTACATTCAGTAGCCCAGCTACTTGTTTACACCCTTGTCTTTTTGCGTACTTATC

GTTTCCTCGGCGGGCTTGCCTGCCGGTTGGACAACTTTATAACCTTTTTAAATCTTCAATCAGCGTCTG

AATAATATACAATAATTACAACTTTCAACAACGGATCTCTTGGTTCTGGCATCGATGAAGAACGCAGCG

AAATGCGATAAGTAGTGTGAATTGCAGAATTCAGTGAATCATCGAATCTTTGAACGCACATTGCGCCC

CTTGGTATTCCATGGGGCATGCCTGTTCGAGCGTCATTTGTACCTTCAAGCTTTGCTTGGTGTTGGGTG

CTTGTCTTTTTGTTAAGACTCACCTCAAAGTCATTGGCAGCCAGTGTTTTGGTAGTAAGCGCAGCACAT

TTTGCGTCTTGGTCCCTTAACAGCAGCATCCATCAAGCCATTTTCTCACTTTTGACCTCGGATCAGGTA

GGGATACCCGCTGAACTTAAGCATATCAAT

Figure S1. ^{1}H NMR spectrum (500 MHz) data for compound **1** in CH_3OH-d_4

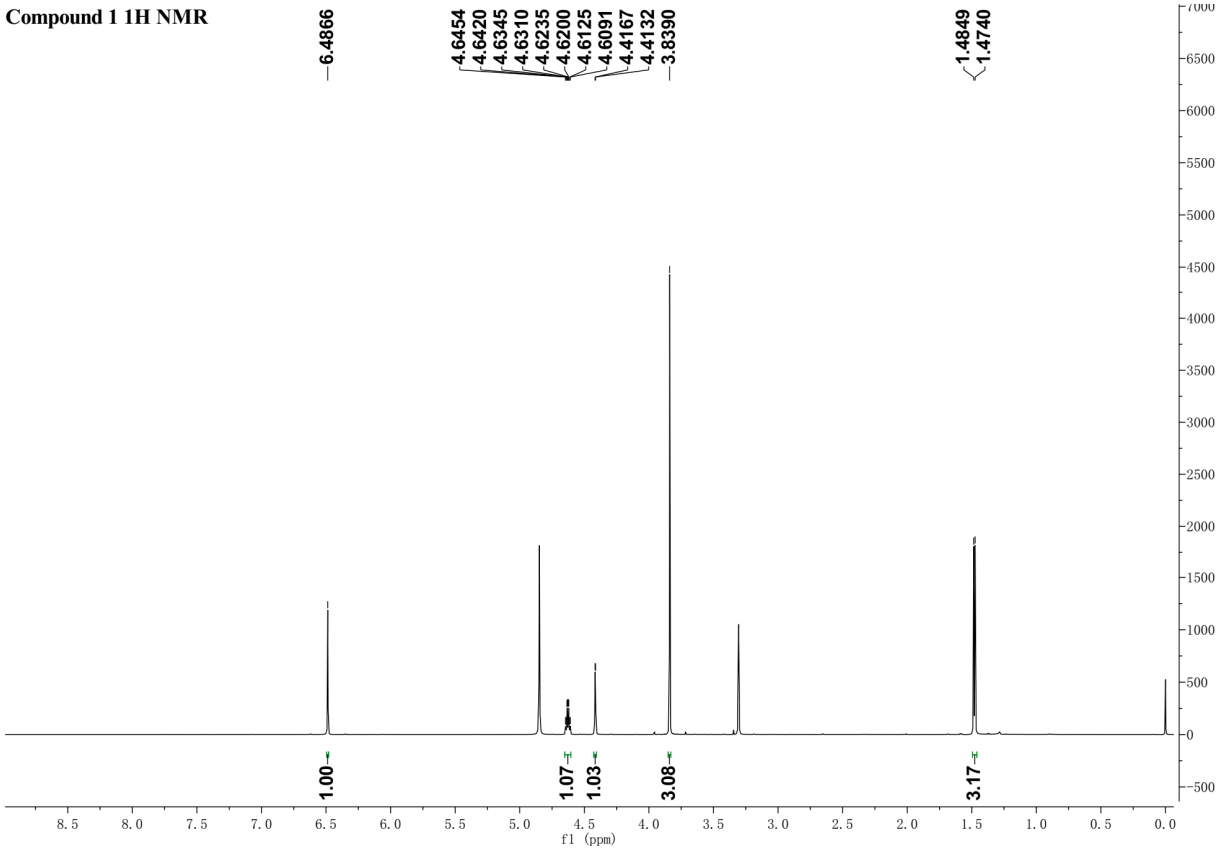

Figure S2. ^{13}C NMR and DEPT135 spectra (125 MHz) of compound **1** in CH_3OH-d_4

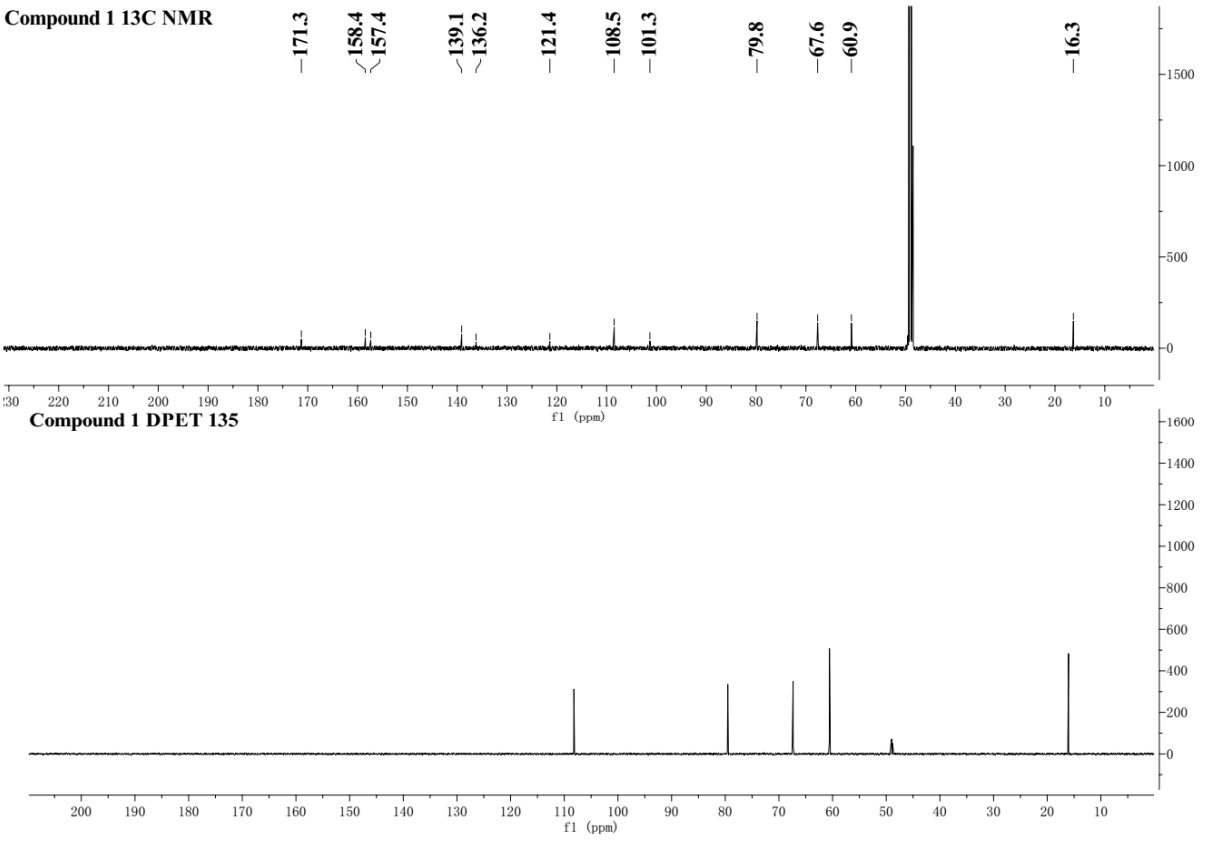

Figure S3. HSQC spectrum (500 MHz) of compound **1** in CH_3OH-d_4

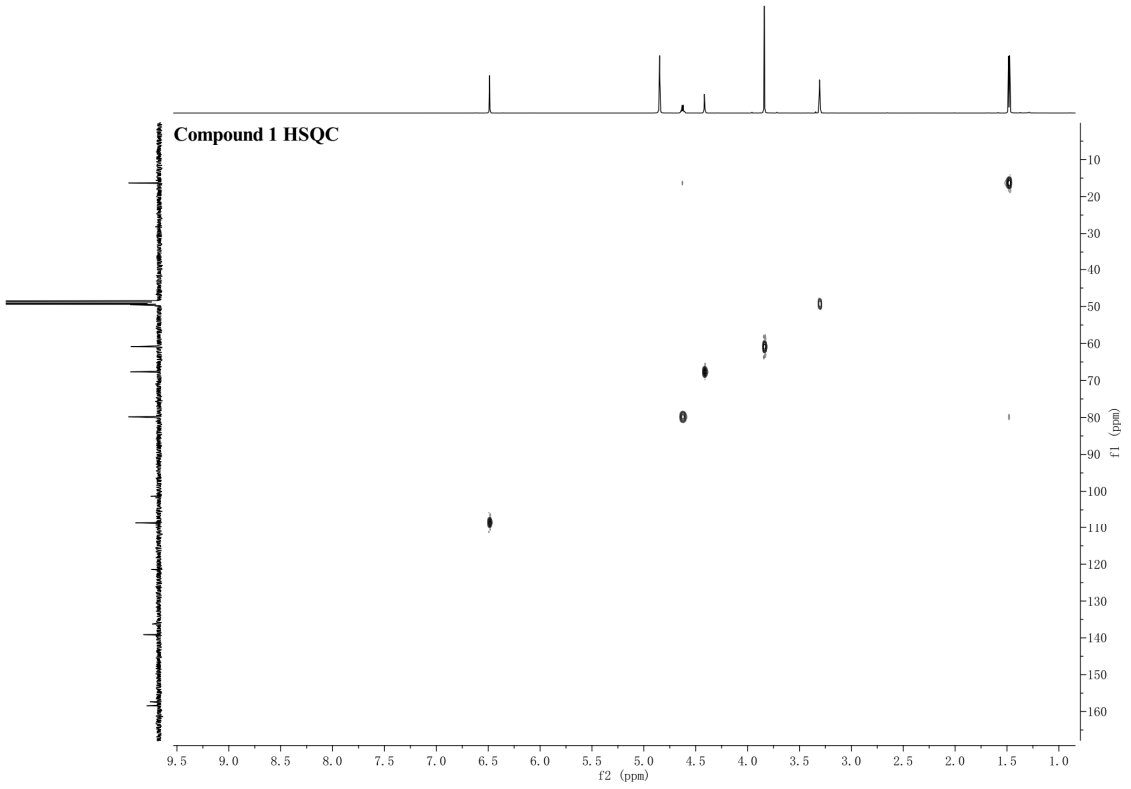

Figure S4. ^1H-^1H COSY spectrum (500 MHz) of compound **1** in CH_3OH-d_4

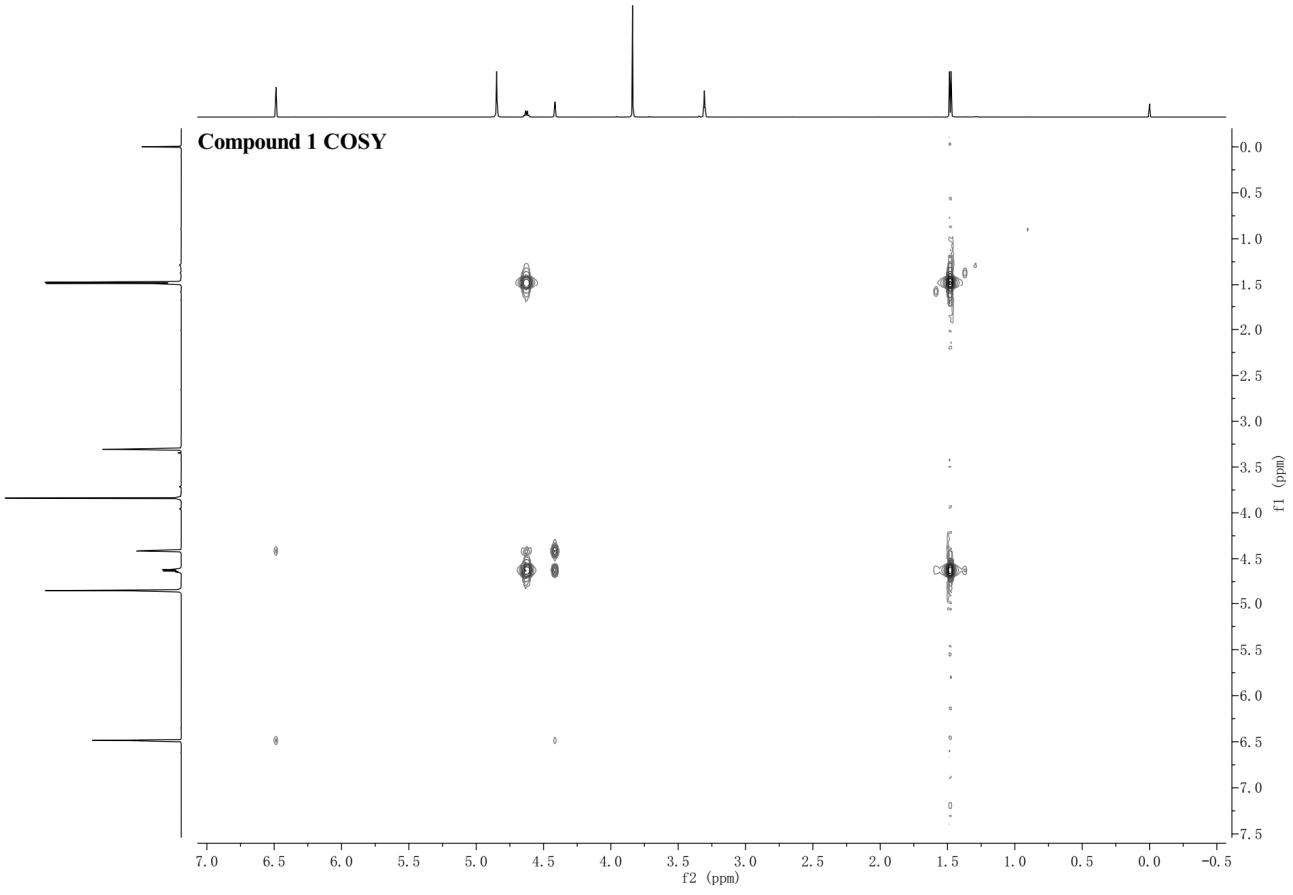

Figure S5. HMBC spectrum (500 MHz) of compound **1** in CH_3OH-d_4

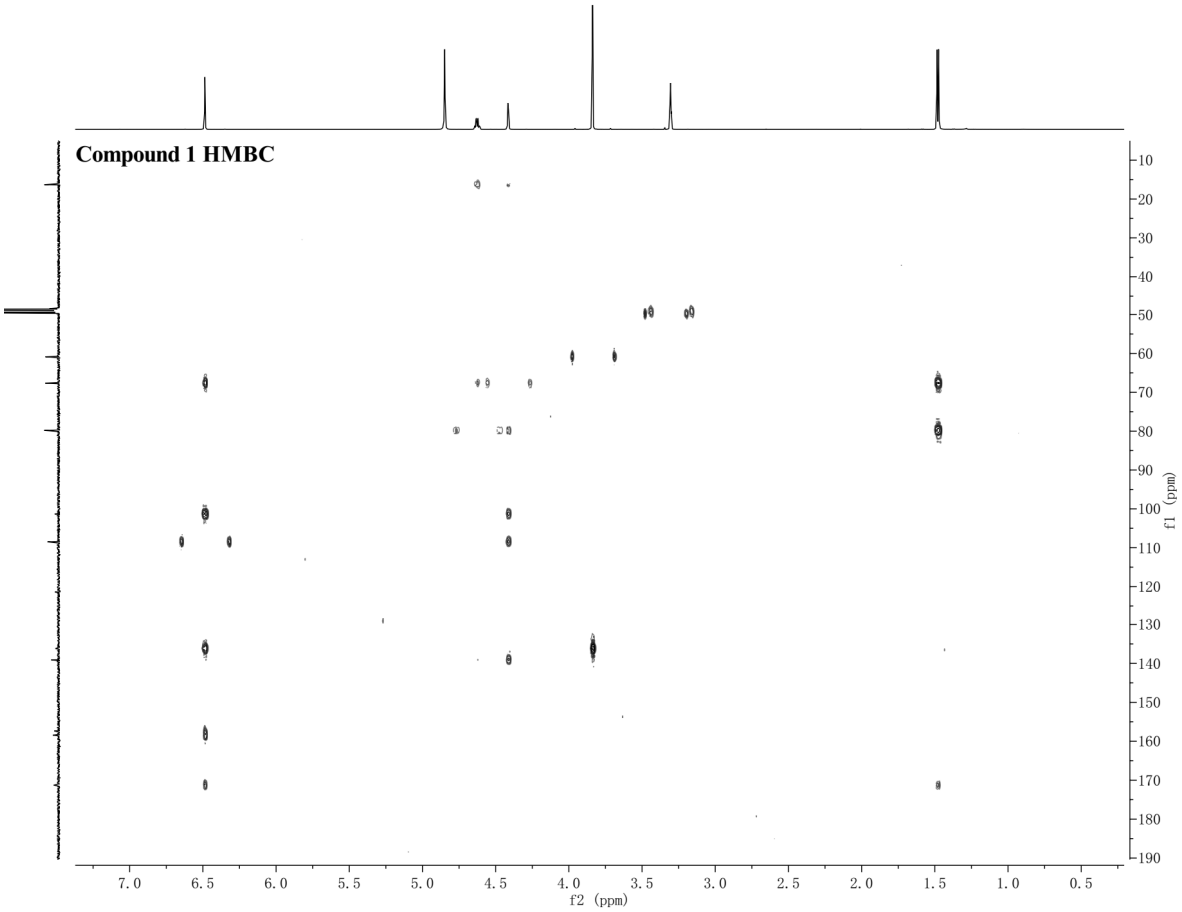

Figure S6. HRESIMS spectrum for compound **1**

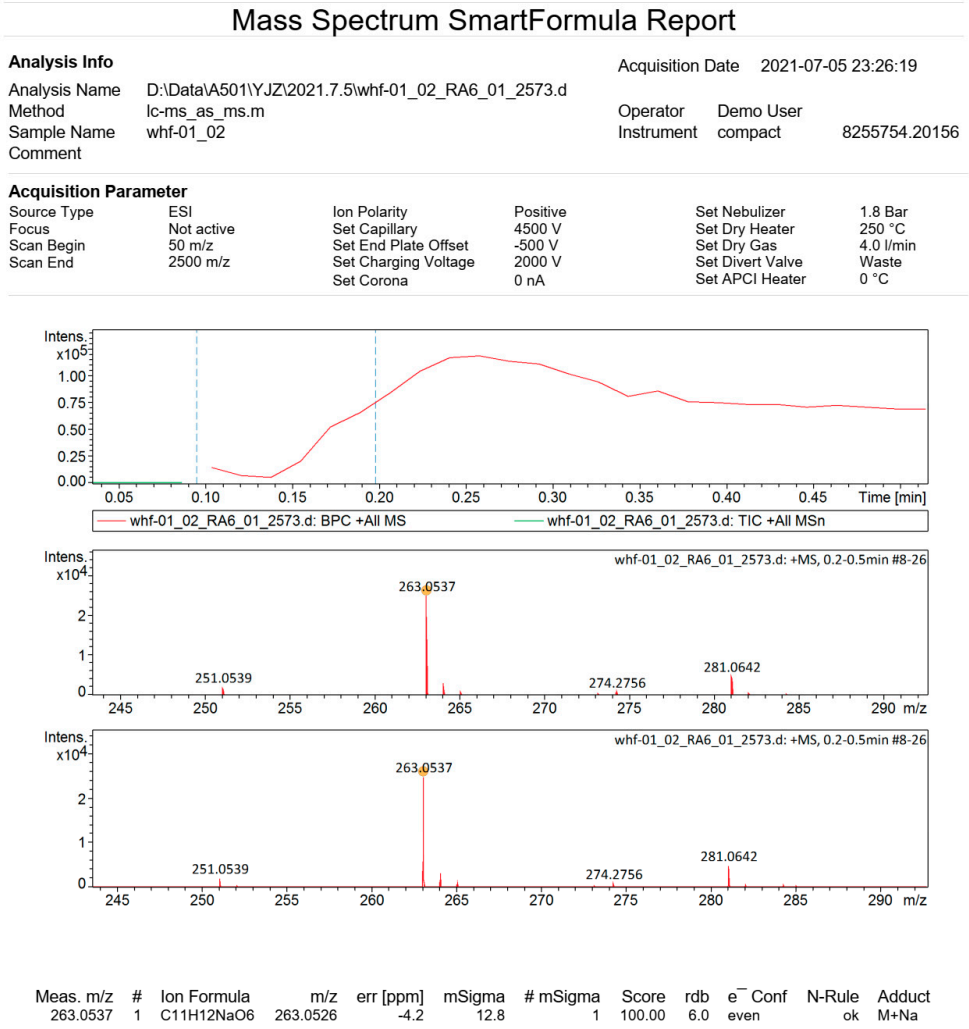

Figure S7. ^{1}H NMR spectrum (500 MHz) data for compound **2** in CH_3OH-d_4

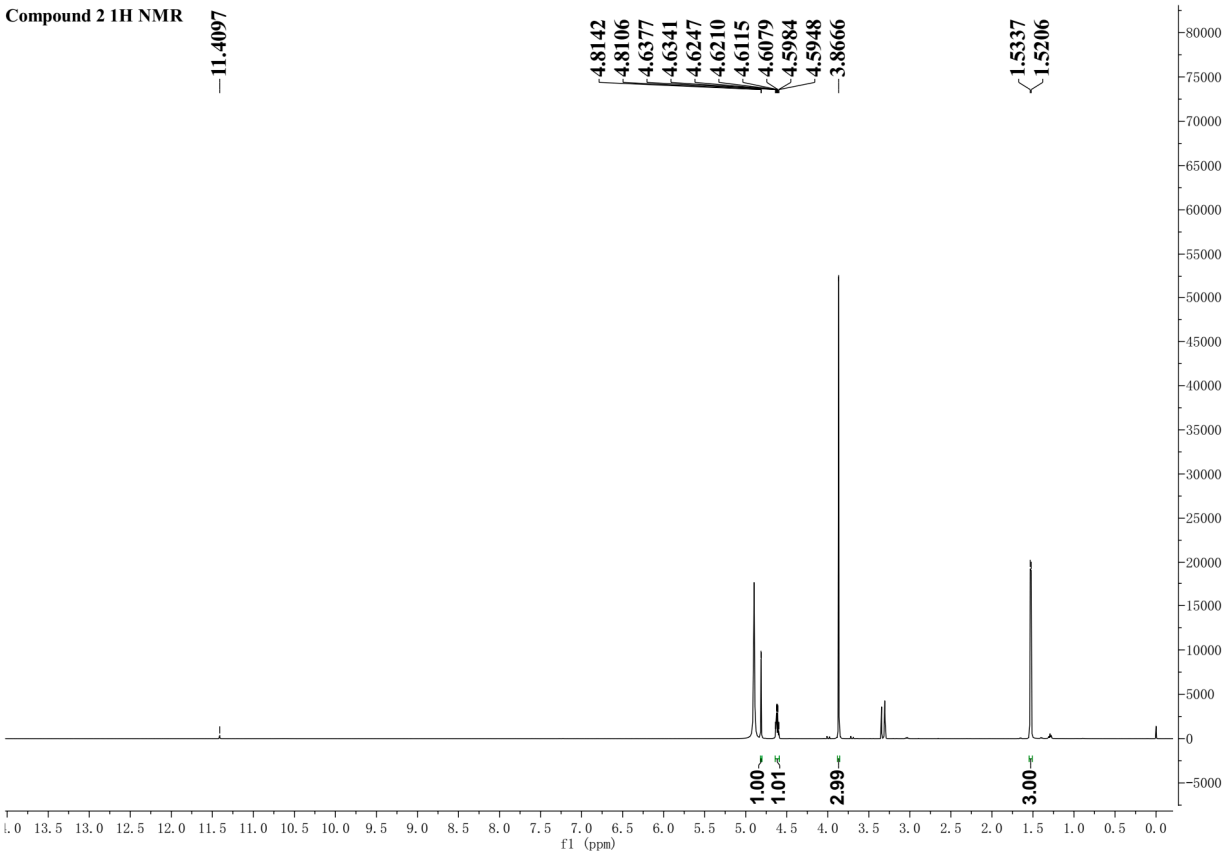

Figure S8. ^{13}C NMR and DEPT135 spectra (125 MHz) data for compound **2** in CH_3OH-d_4

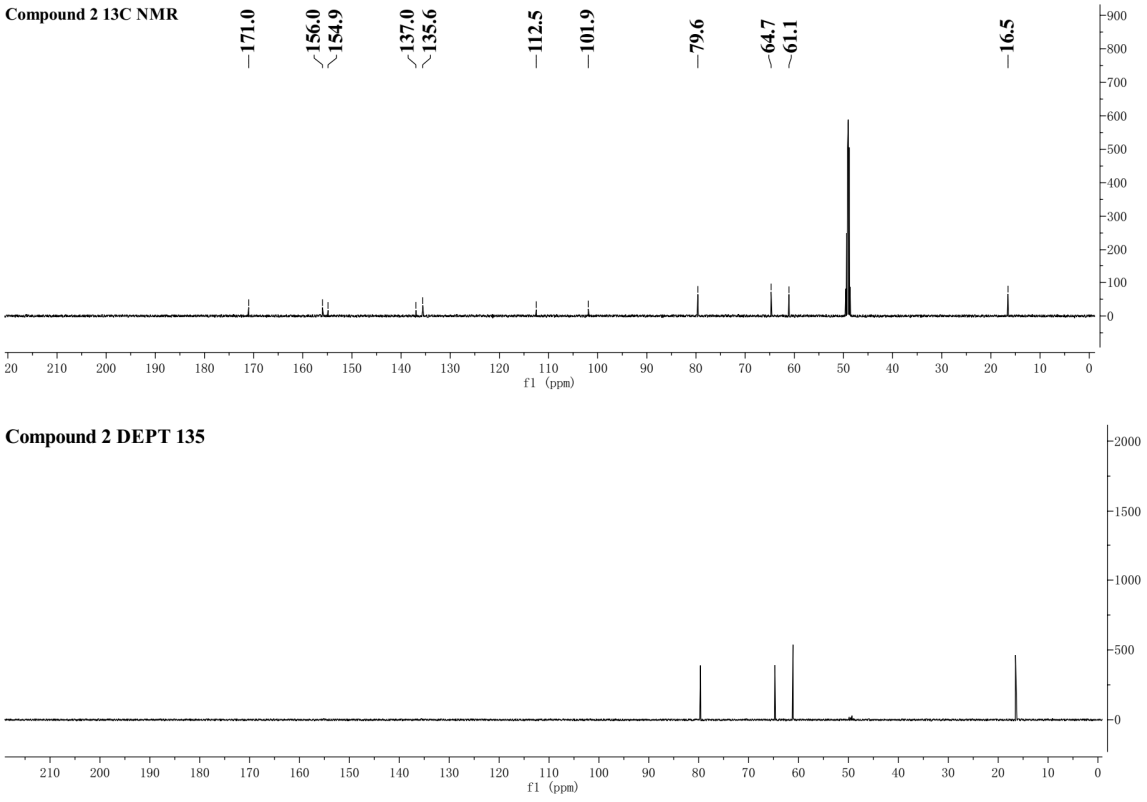

Figure S9. HSQC spectrum (500 MHz) of compound **2** in CH_3OH-d_4

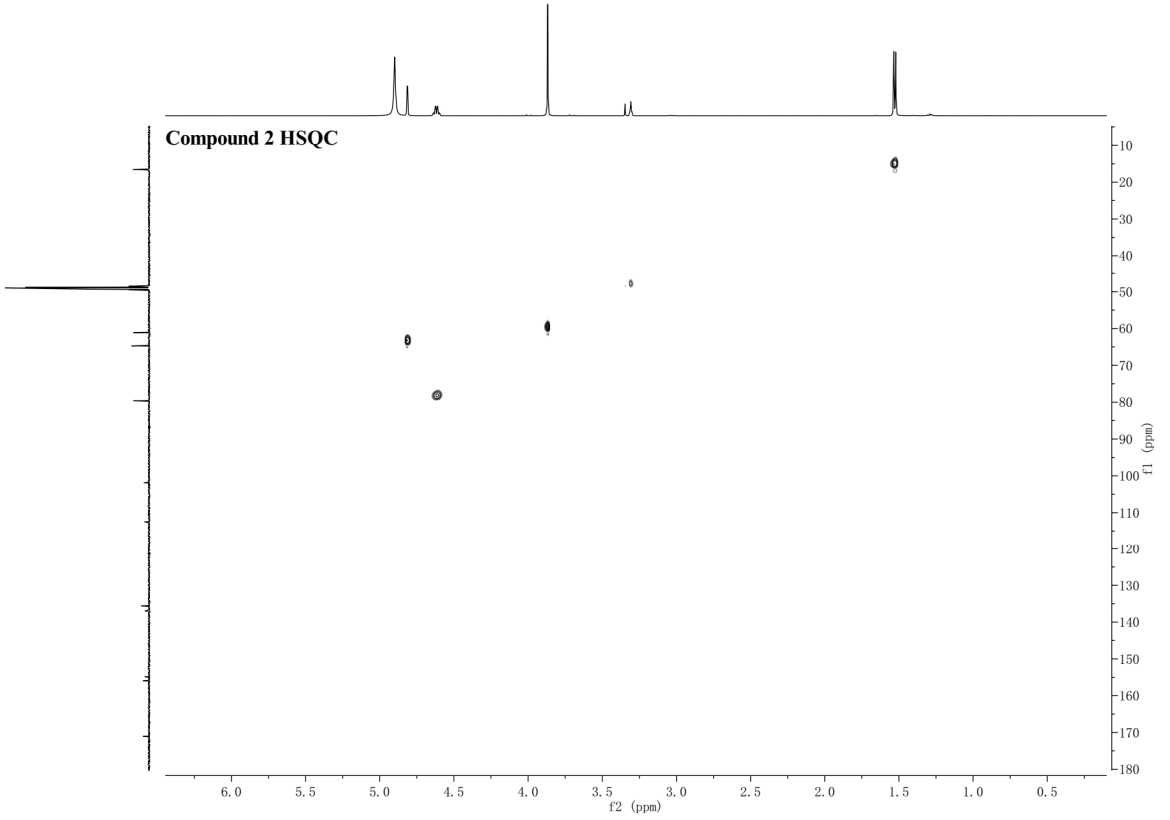

Figure S10. ^1H-^1H COSY spectrum (500 MHz) of compound **2** in CH_3OH-d_4

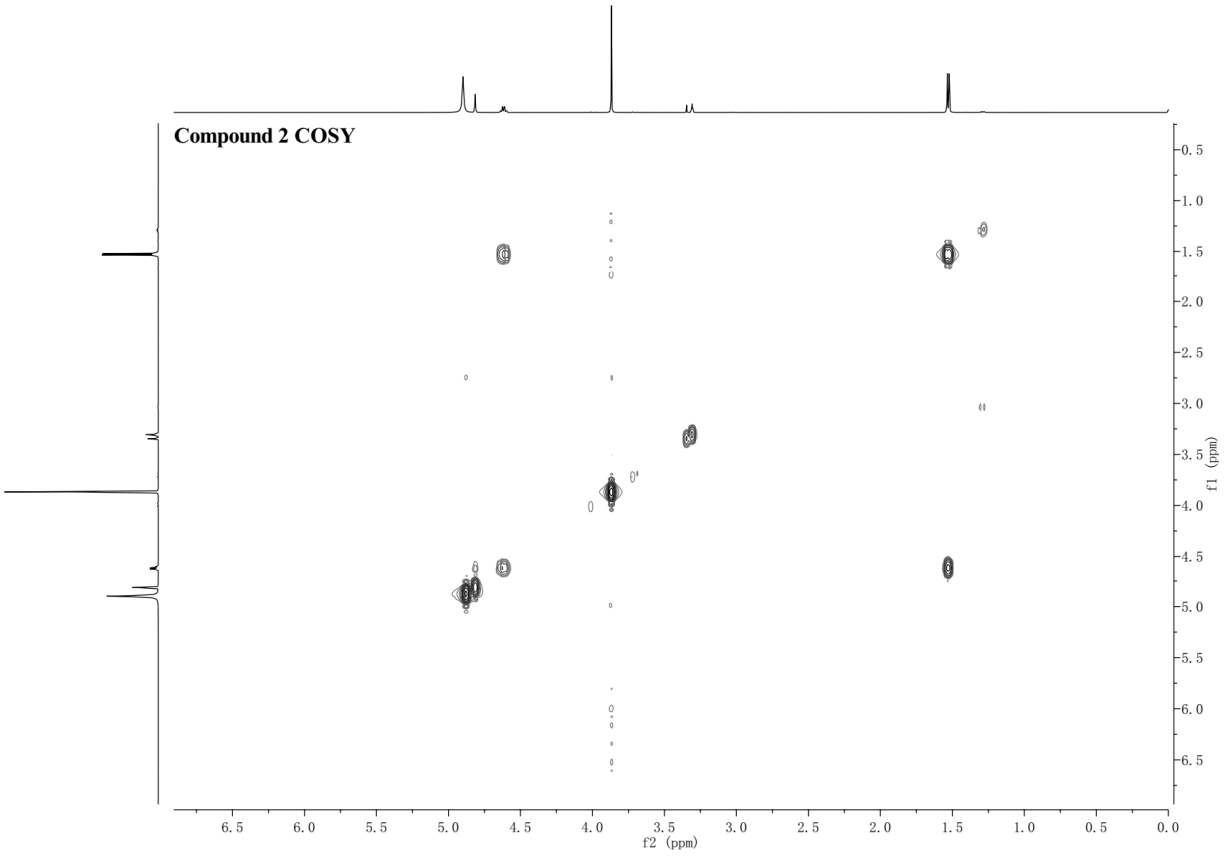

Figure S11. HMBC spectrum (500 MHz) of compound **2** in CH_3OH-d_4

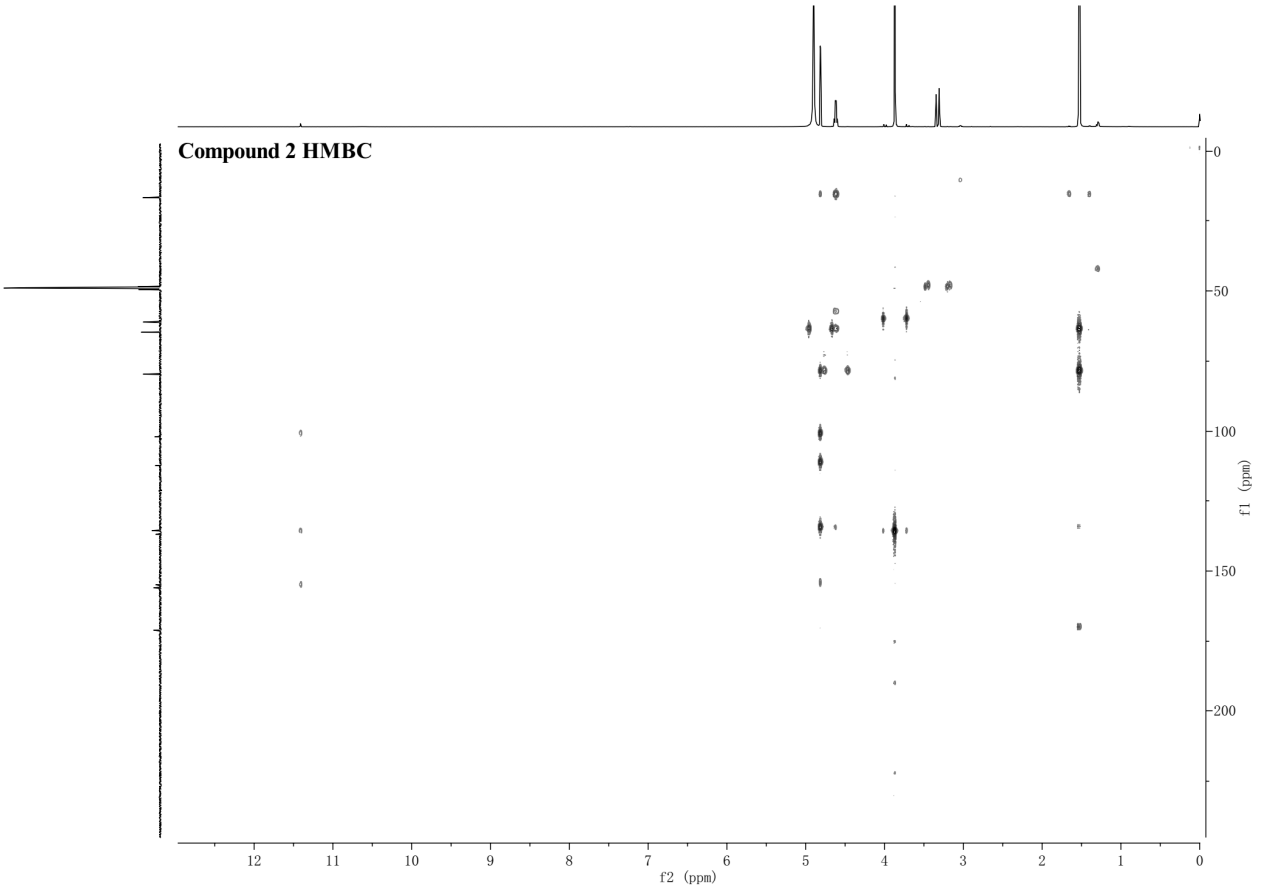

Figure S12. HRESIMS spectrum for compound **2**

Mass Spectrum SmartFormula Report

Analysis Info

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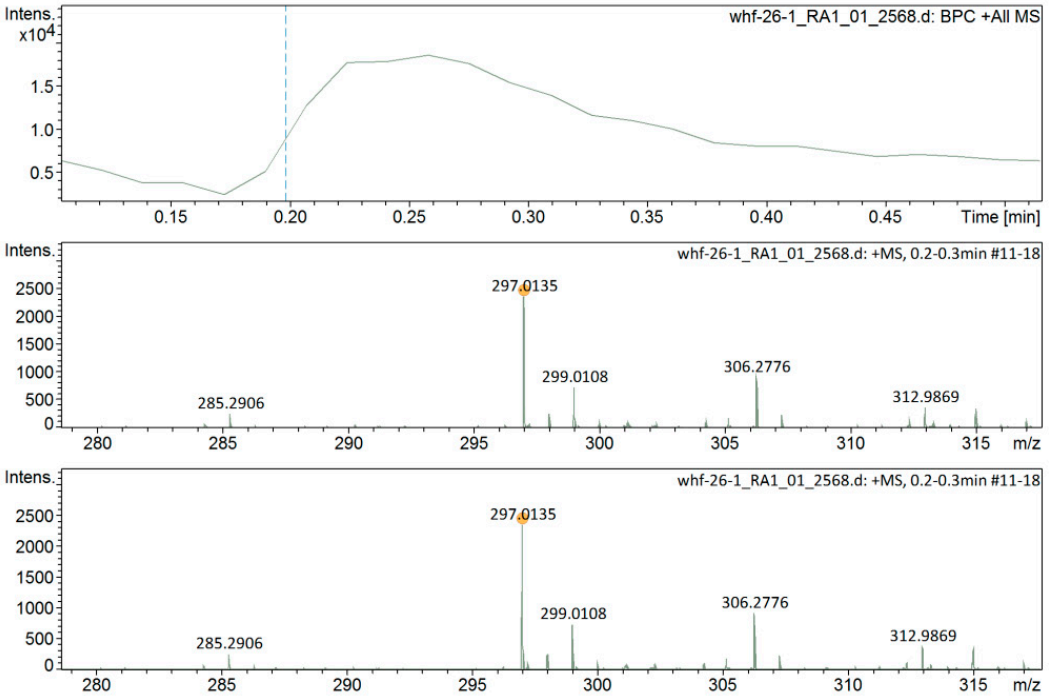
Sample Name	whf-26-1	Operator	Demo User
Comment		Instrument	compact 8255754.20156

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	250 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	Adduct
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whf-26-1_RA1_01_2568.d

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Figure S13. ^{1}H NMR spectrum (500 MHz) data for compound **3** in CH_3OH-d_4

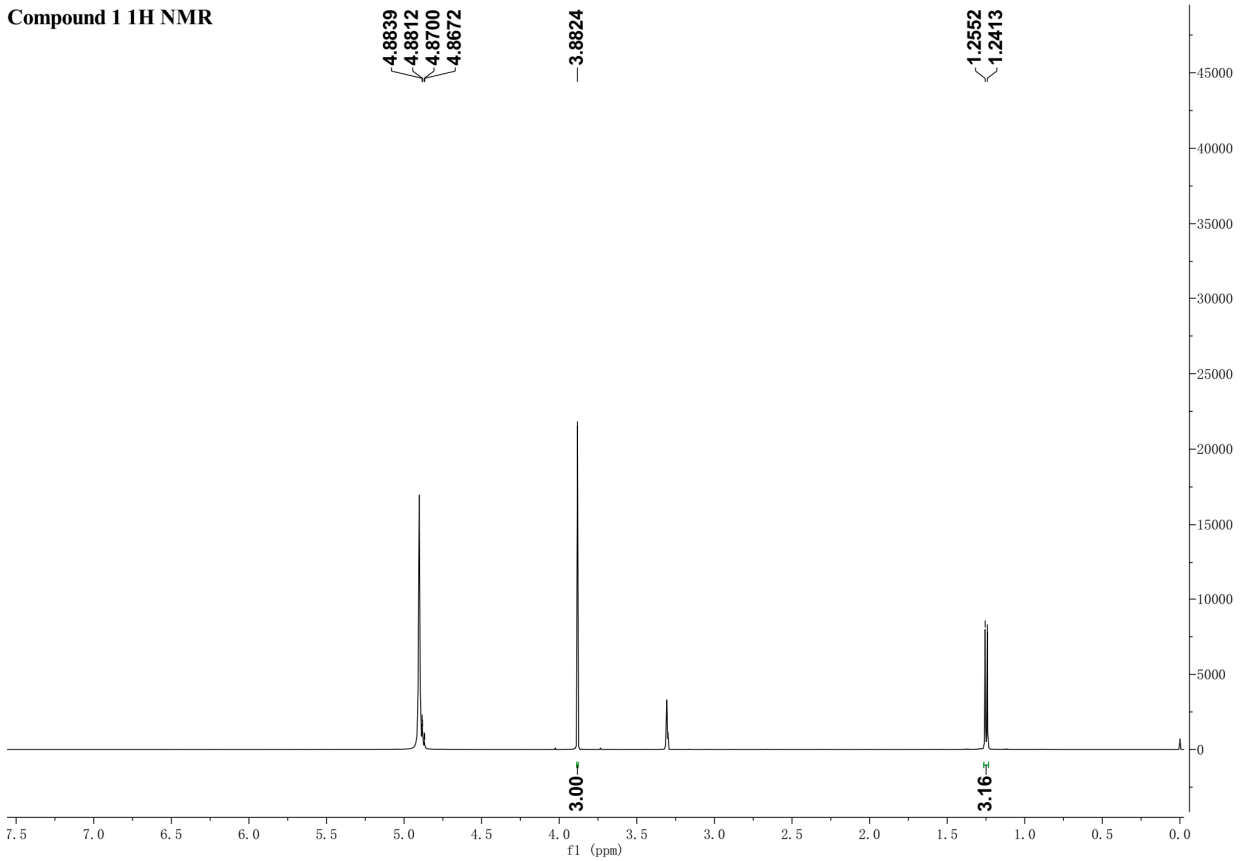

Figure S14. ^{13}C NMR and DEPT135 spectra (125 MHz) data for compound **3** in CH_3OH-d_4

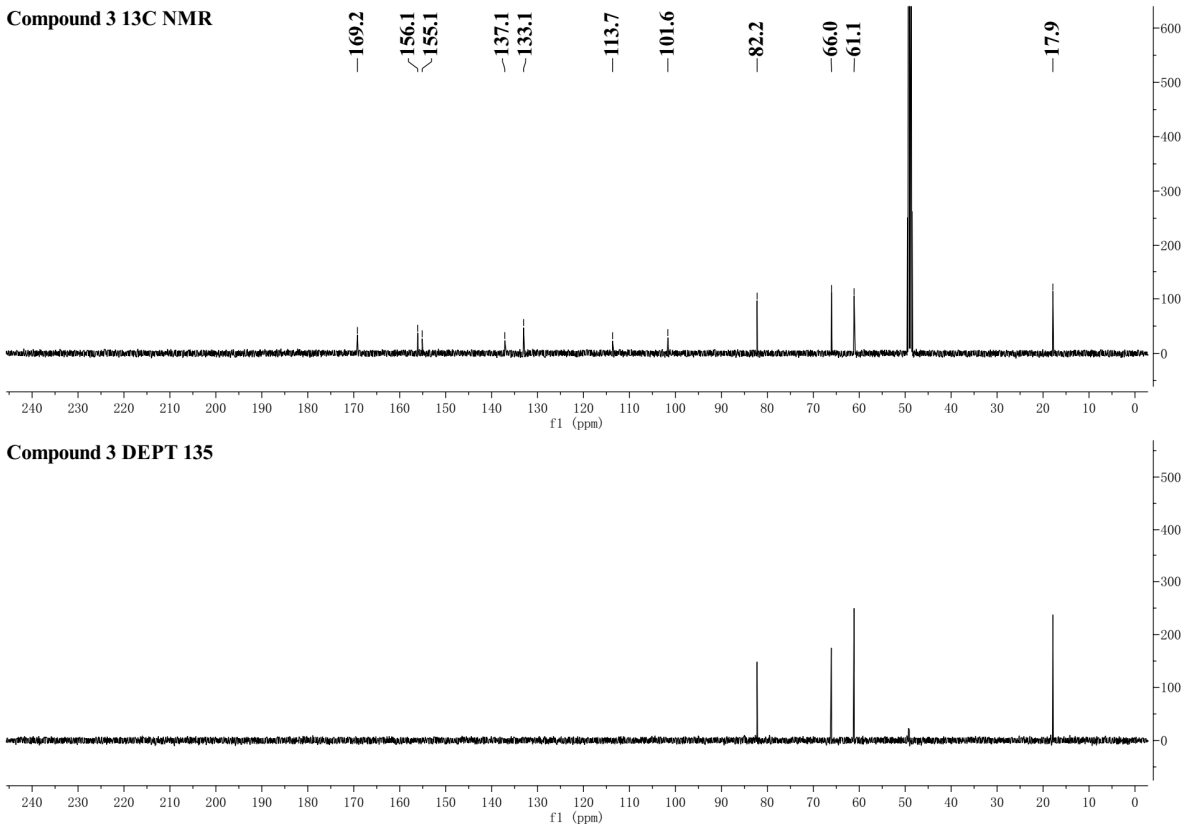

Figure S15. HSQC spectrum (500 MHz) of compound **3** in CH_3OH-d_4

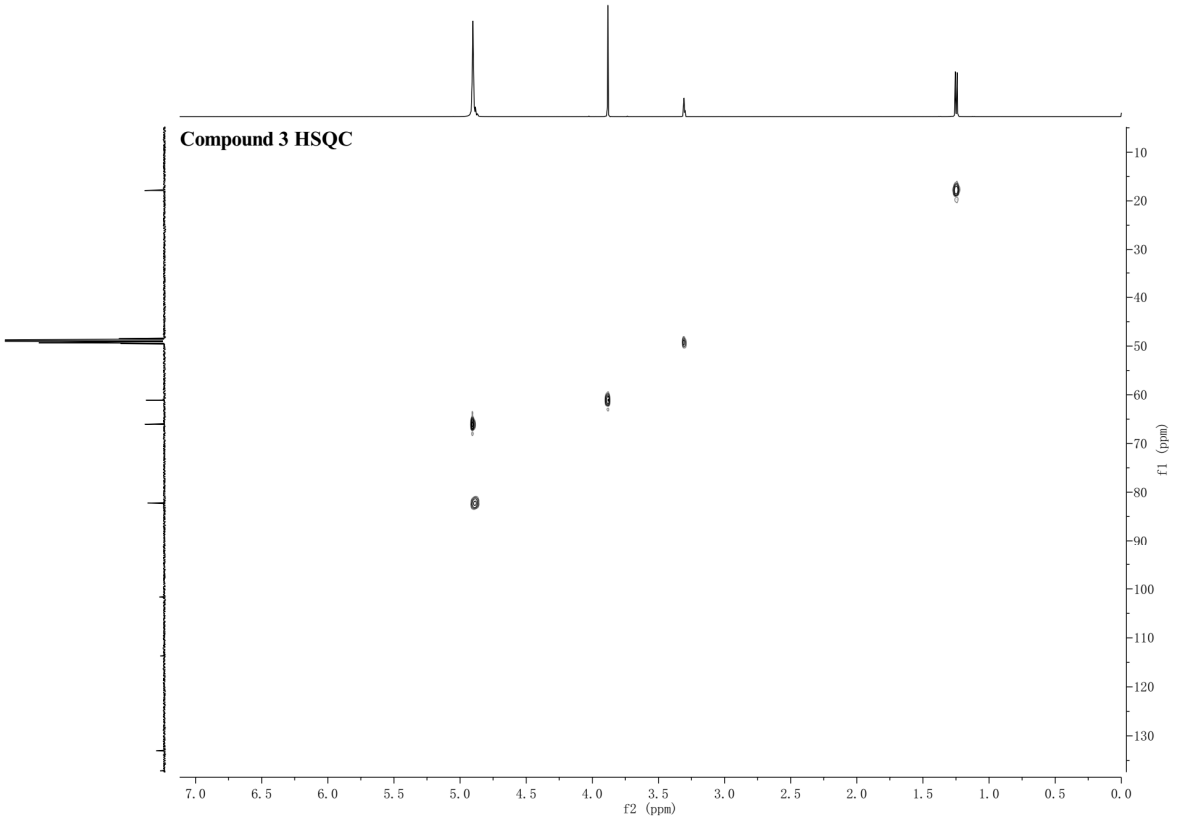

Figure S16. ^1H-^1H COSY spectrum (500 MHz) of compound **3** in CH_3OH-d_4

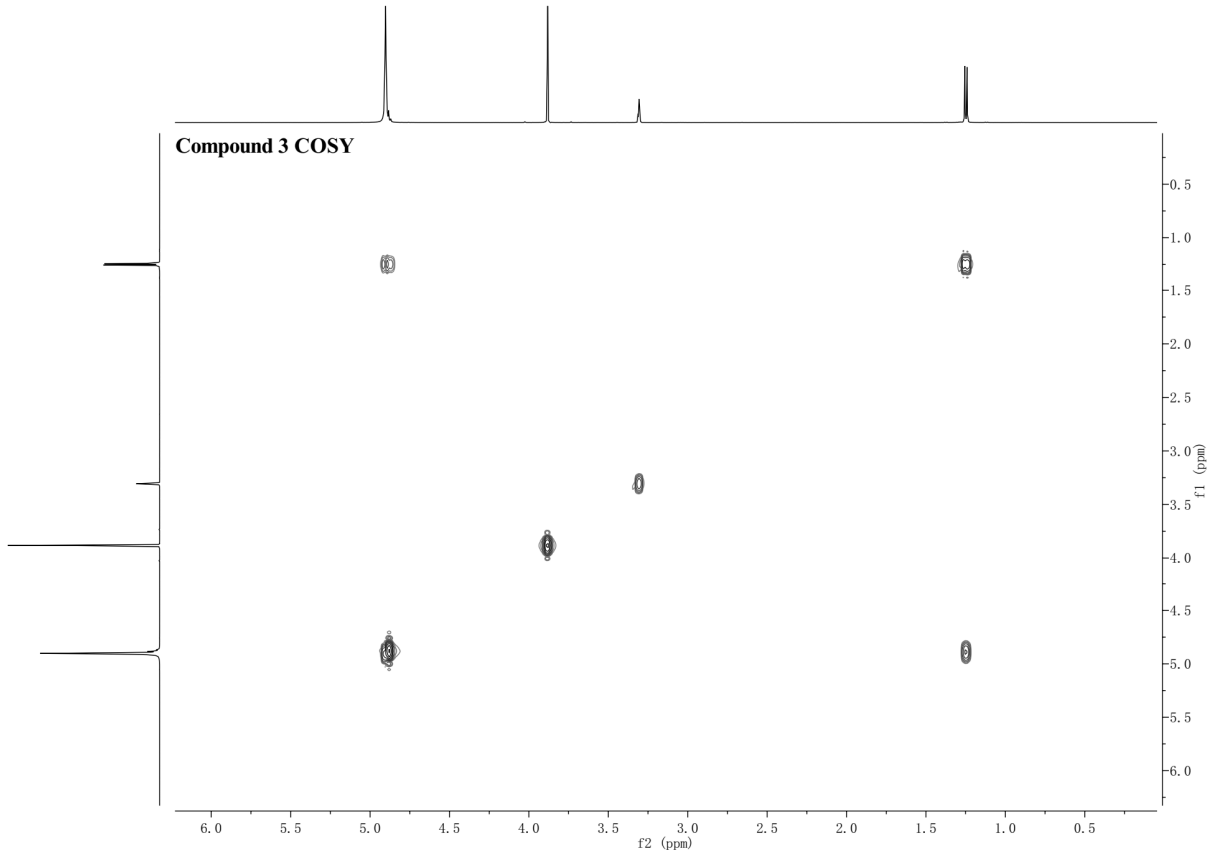

Figure S17. HMBC spectrum (500 MHz) of compound **3** in CH_3OH-d_4

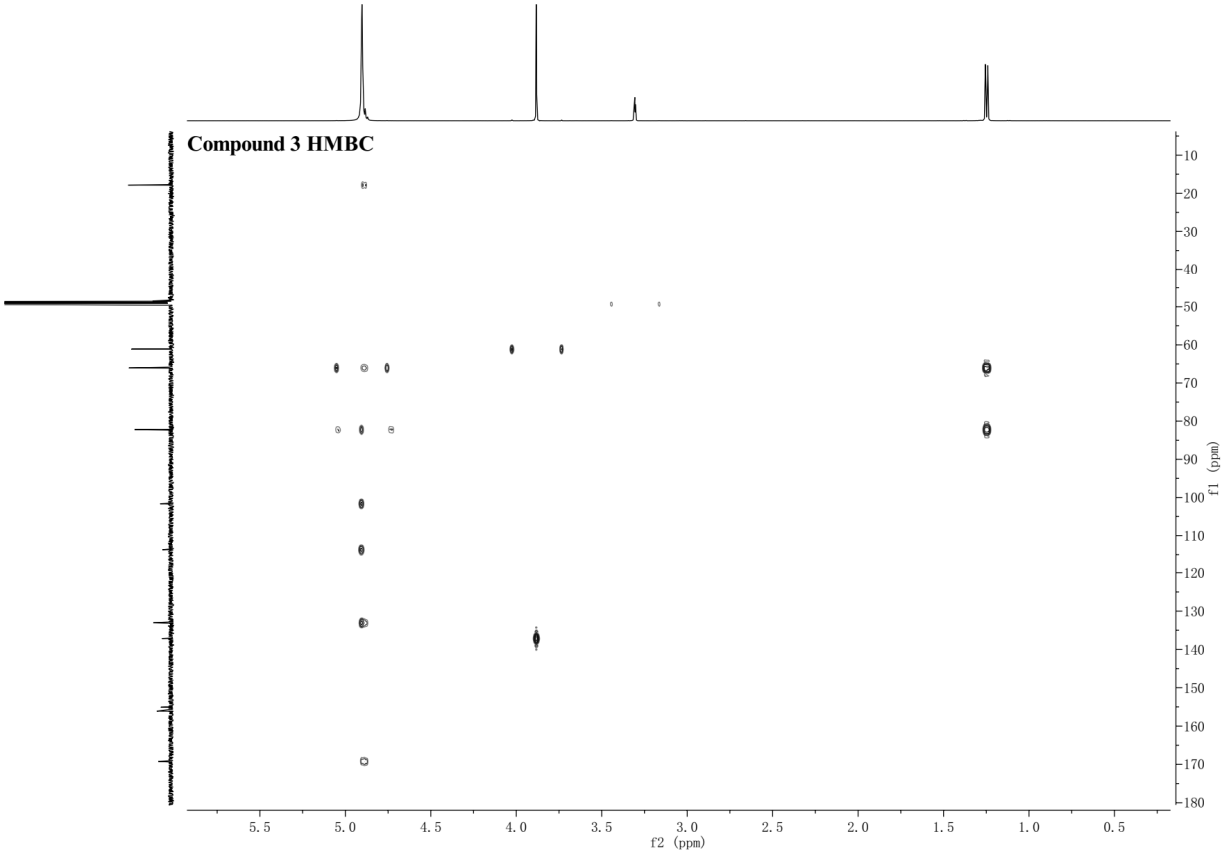

Figure S18. ROESY spectrum (500 MHz) of compound **3** in CH_3OH-d_4

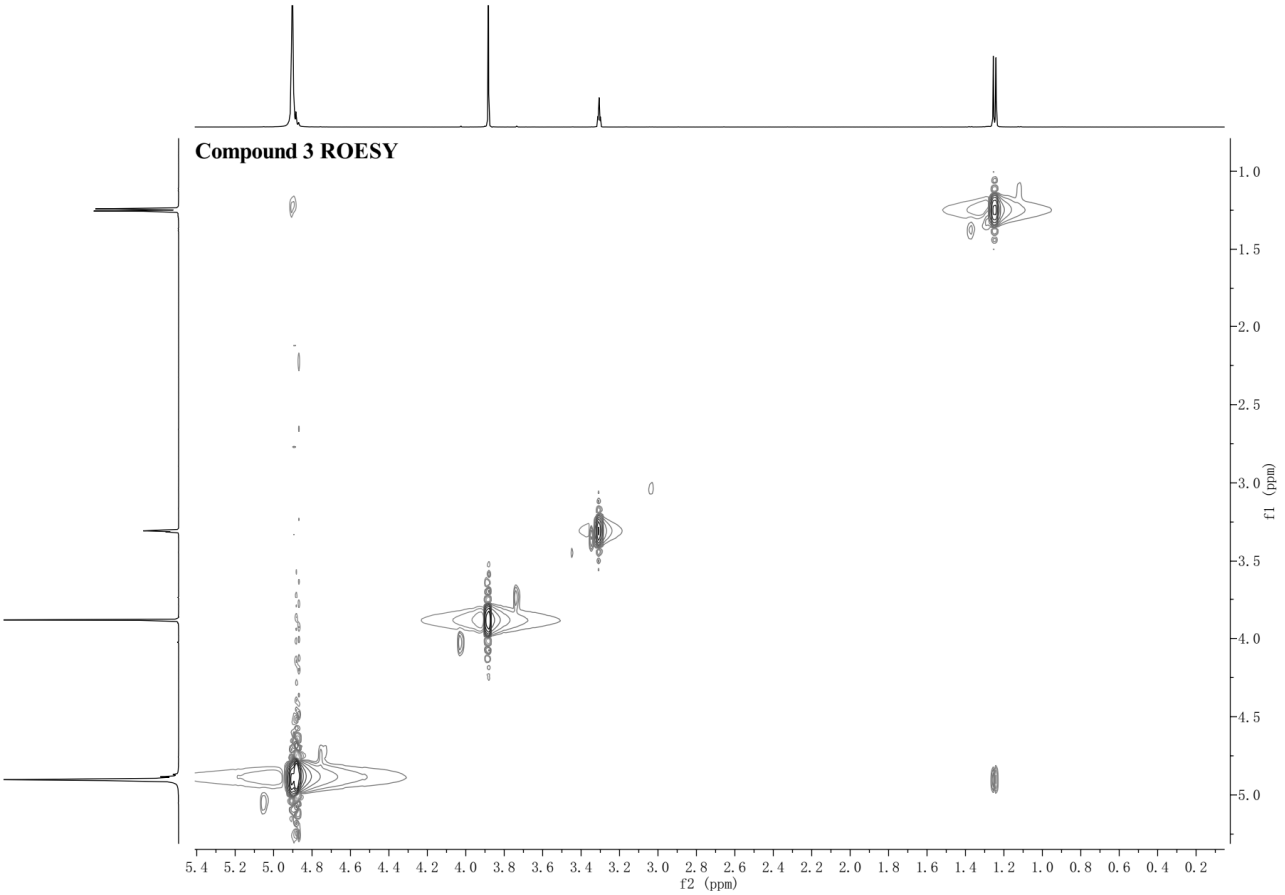

Figure S19. 1D NOESY spectrum (500 MHz) of compound **3** in CH_3OH-d_4

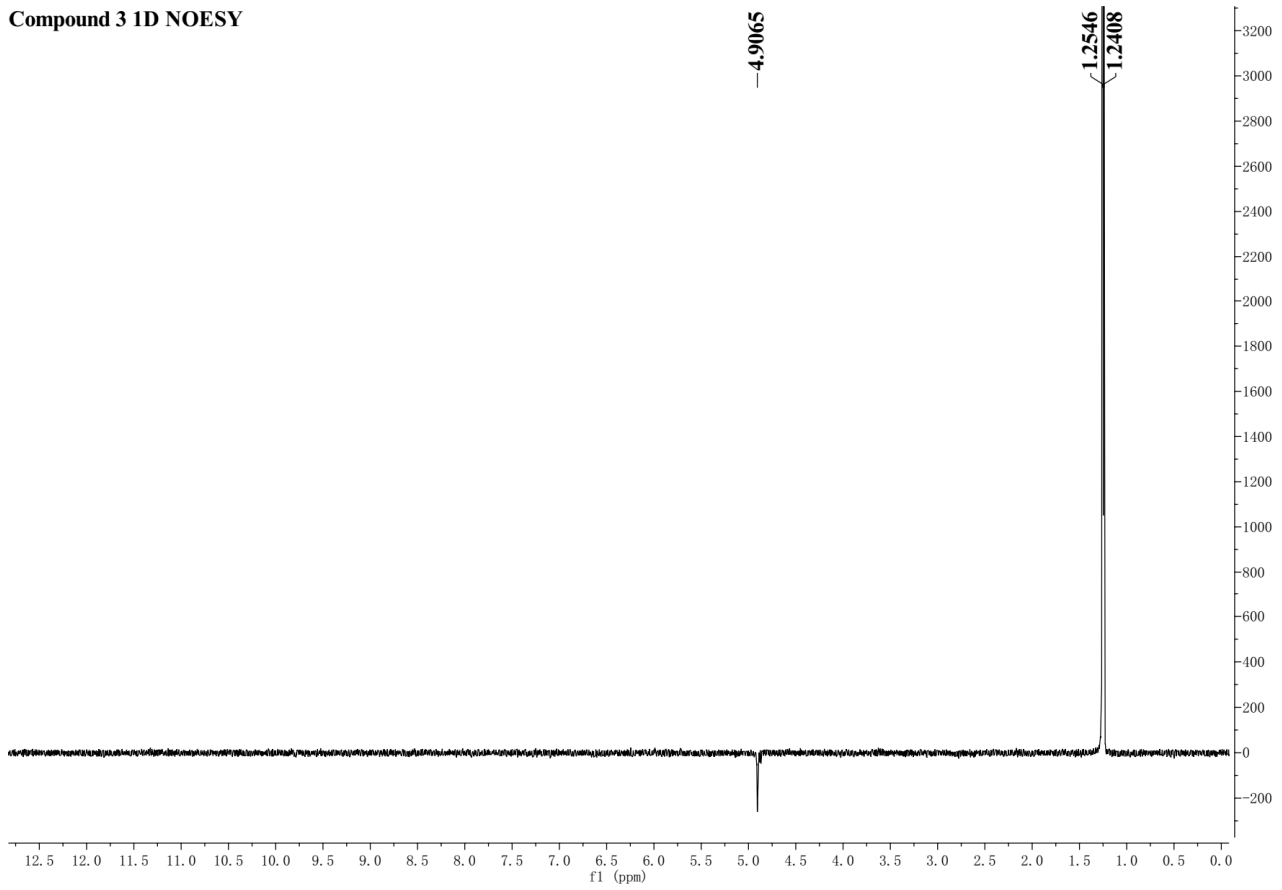

Figure S 20. HRESIMS spectrum for compound **3**

Mass Spectrum SmartFormula Report

Analysis Info

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Sample Name	whf-26-02	Instrument	compact 8255754.20156
Comment			

Acquisition Parameter

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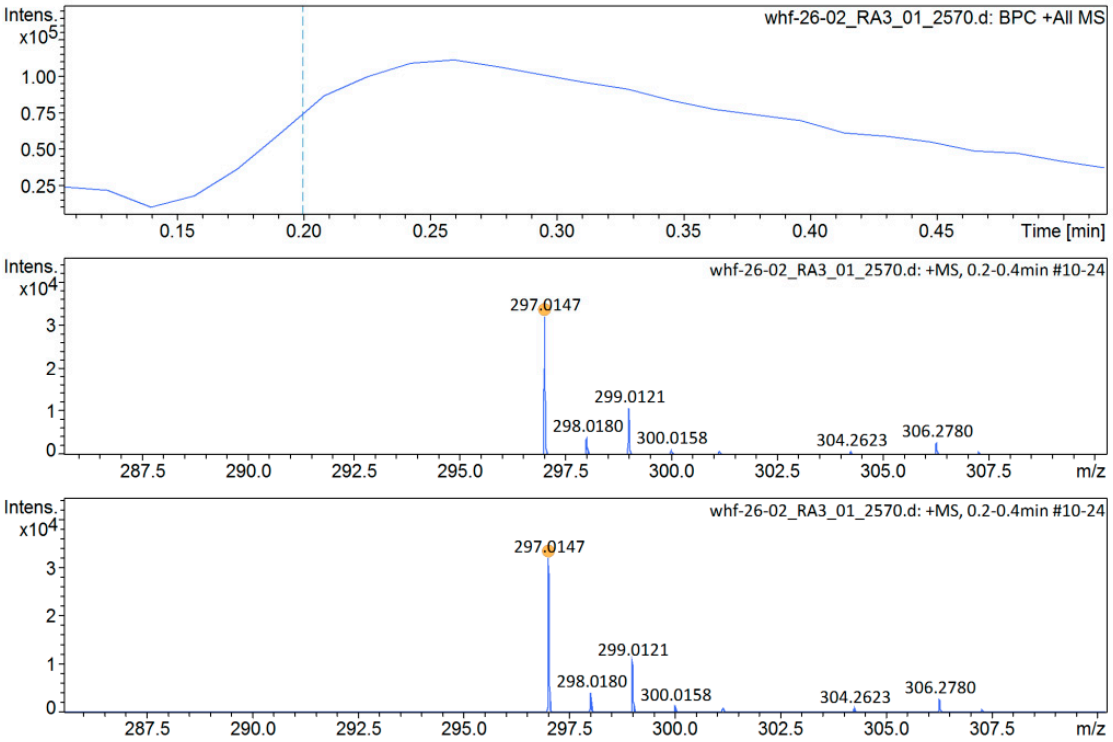
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	Adduct
297.0147	1	C11H11ClNaO6	297.0136	-3.4	4.4	1	100.00	6.0	even	ok	M+Na

Figure S21. ^{1}H NMR spectrum (600 MHz) data for compound **4** in CH_3OH-d_4

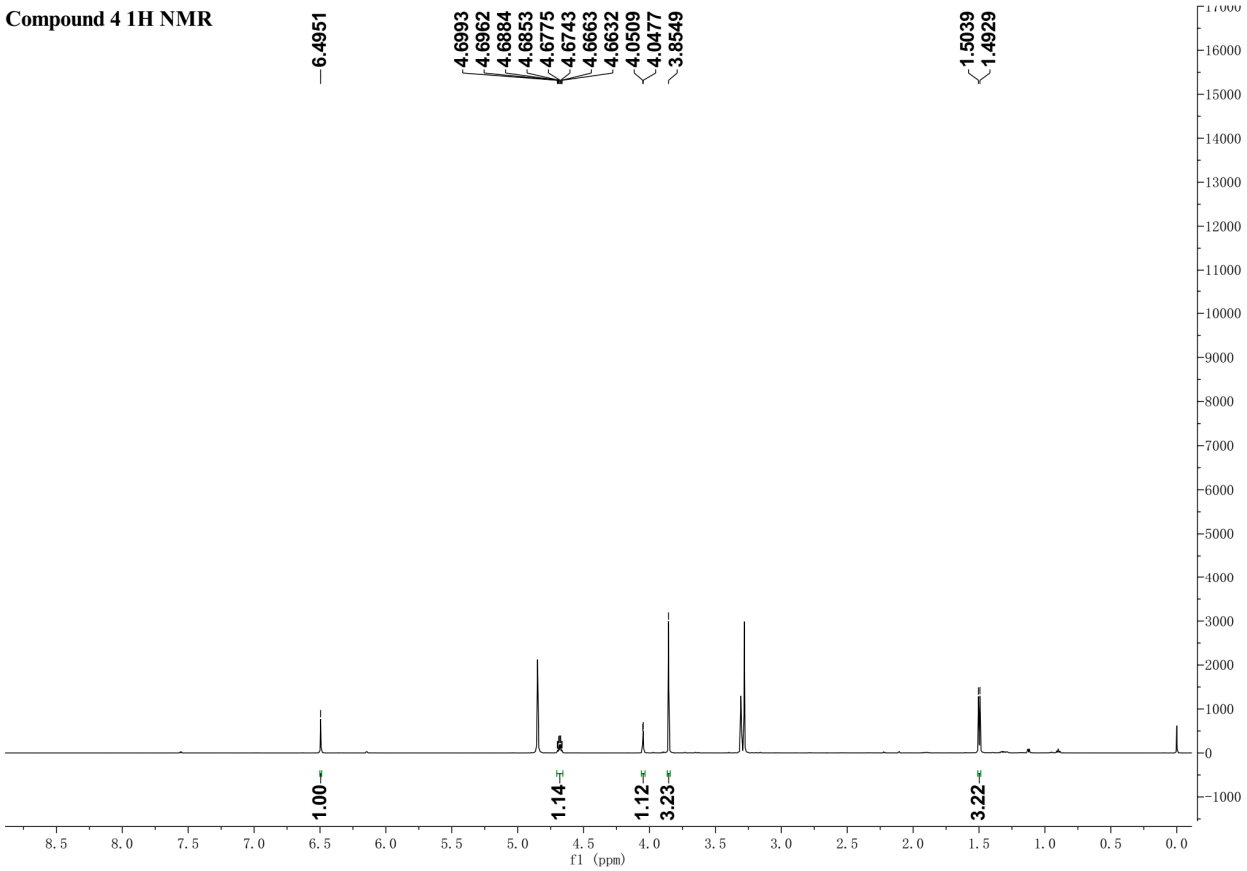


Figure S22. ^{13}C NMR and DEPT135 spectra (150 MHz) data for compound **4** in CH_3OH-d_4

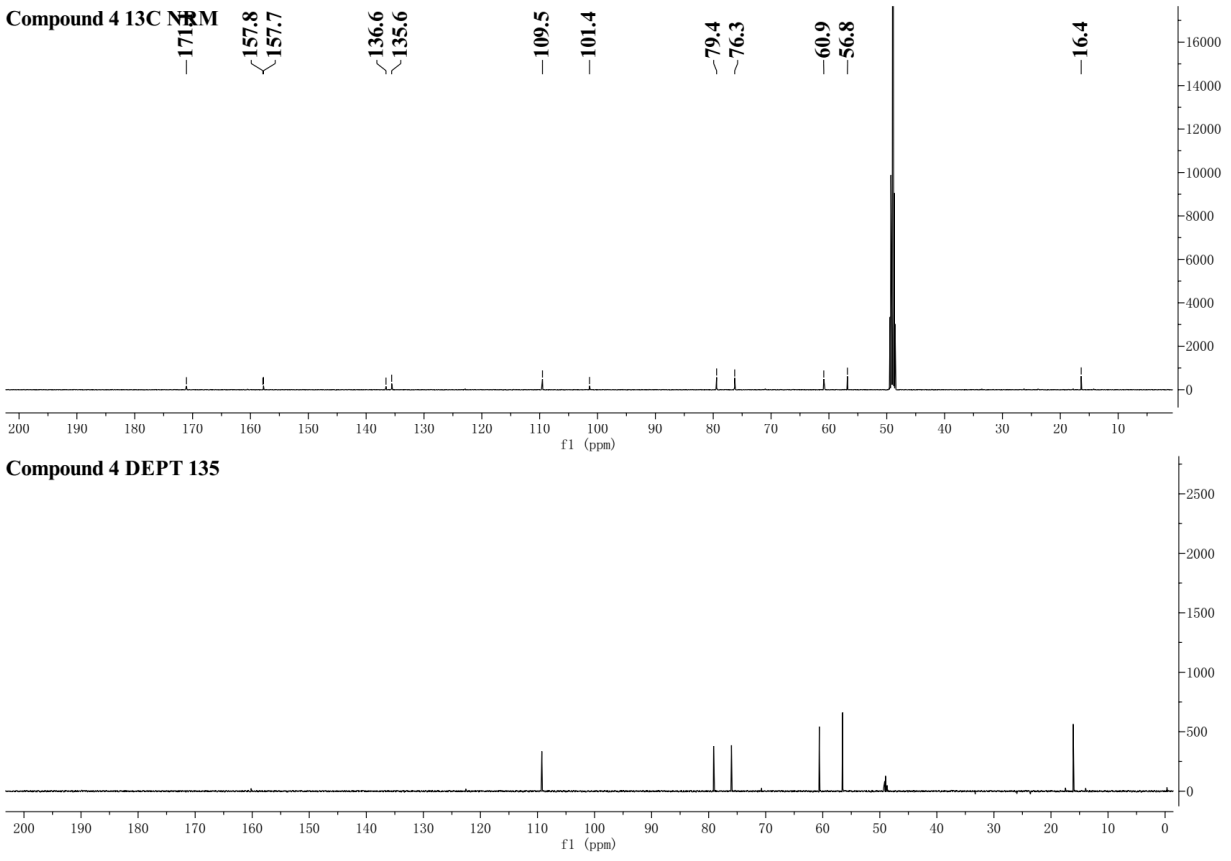


Figure S23. HSQC spectrum (600 MHz) of compound **4** in CH_3OH-d_4

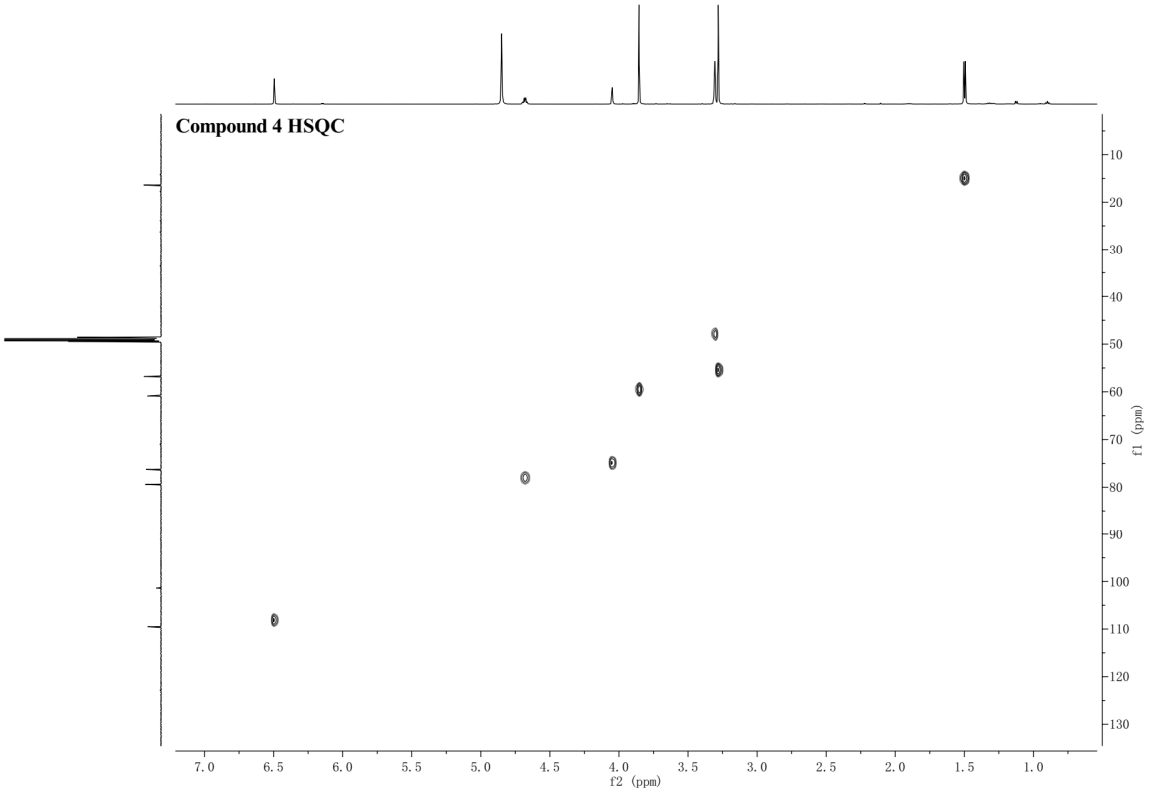


Figure S24. ^1H-^1H COSY spectrum (600 MHz) of compound **4** in CH_3OH-d_4

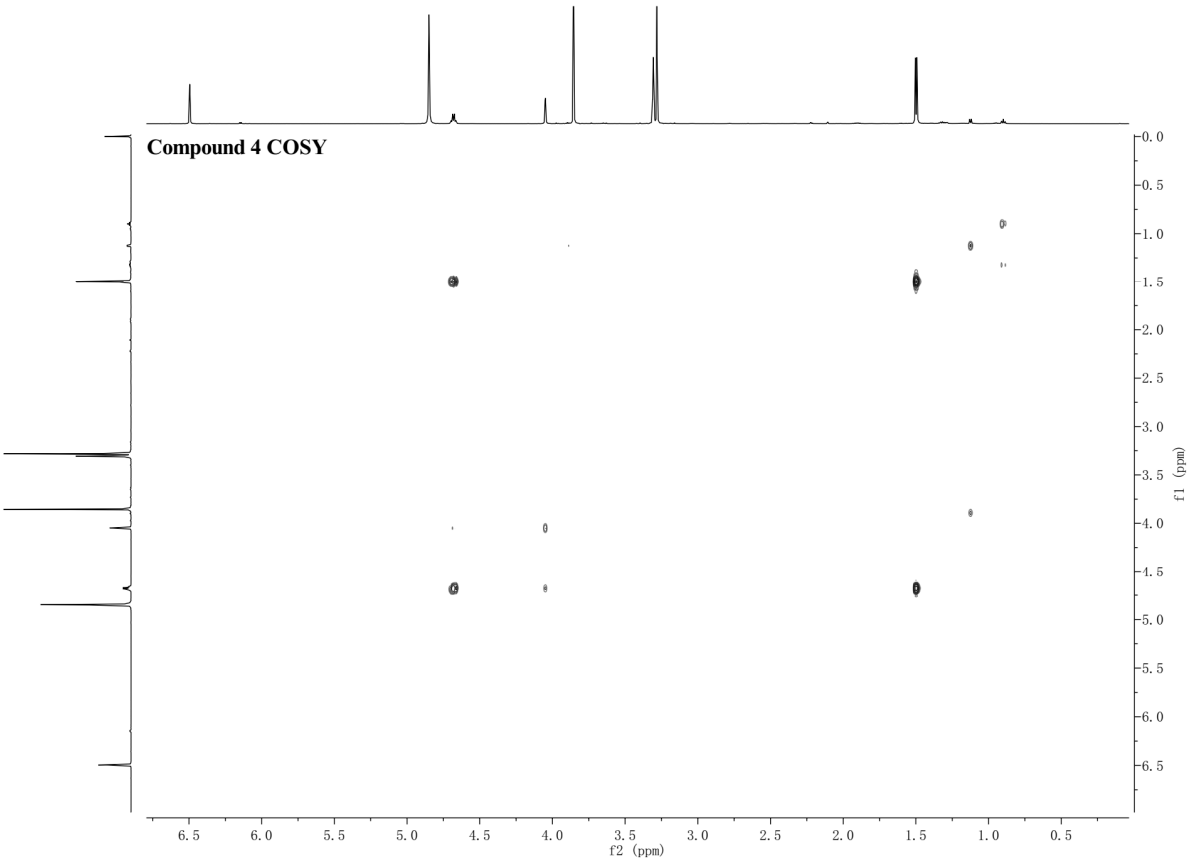


Figure S25. HMBC spectrum (600 MHz) of compound **4** in CH_3OH-d_4

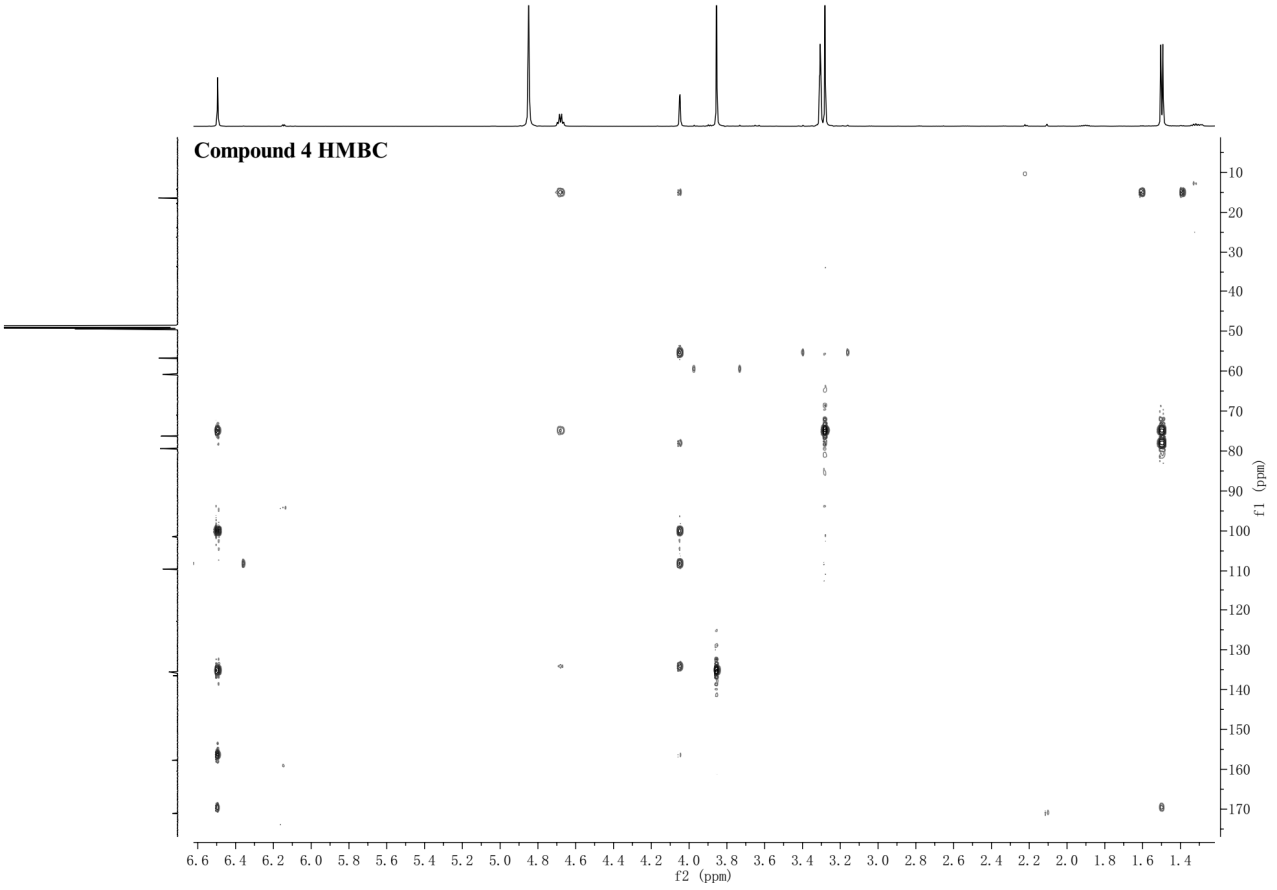


Figure S26. HRESIMS spectrum for compound **4**

Mass Spectrum SmartFormula Report

Analysis Info

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Sample Name	WHF-24	Instrument	compact 8255754.20156
Comment			

Acquisition Parameter

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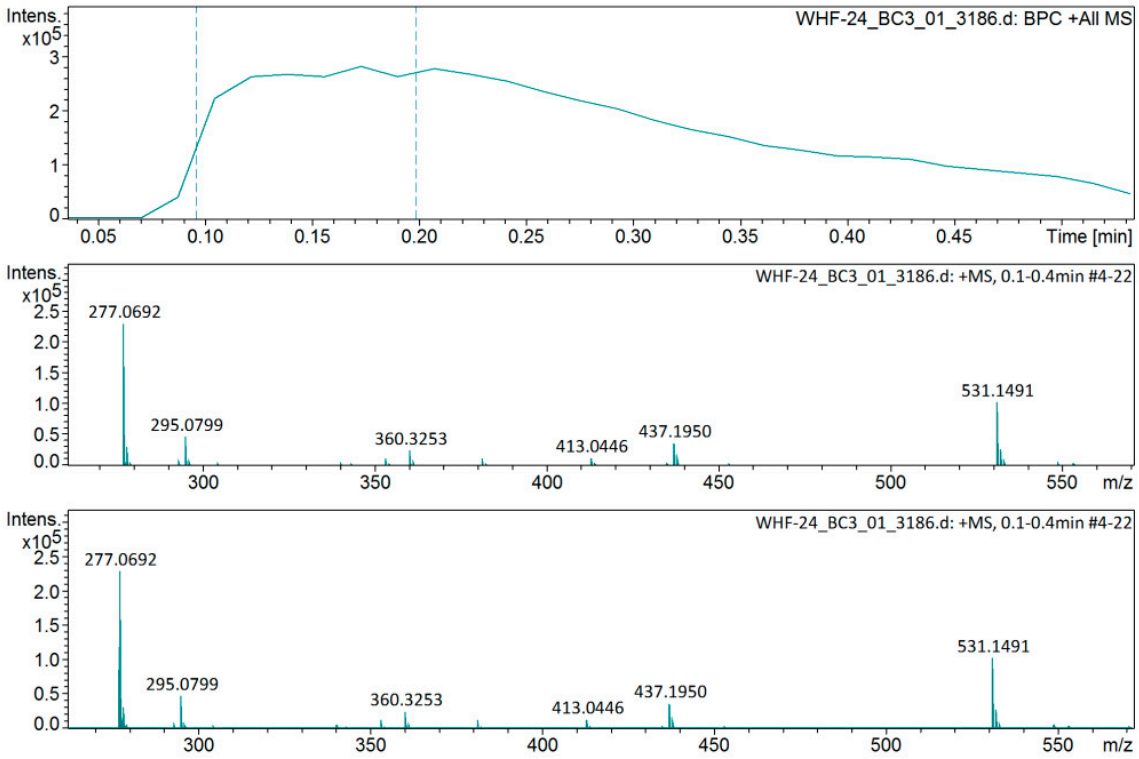
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



WHF-24_BC3_01_3186.d

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Figure S27. ^{1}H NMR spectrum (600 MHz) data for compound **5** in CH_3OH-d_4

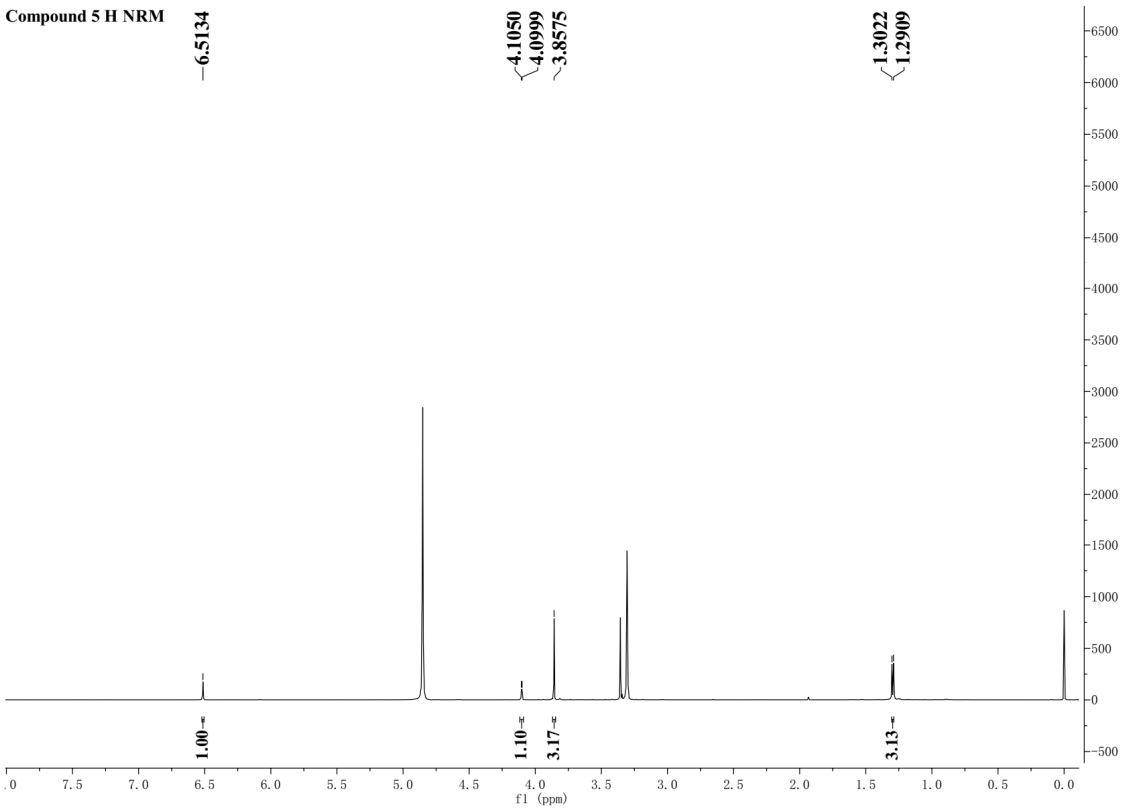


Figure S28. ^{13}C NMR and DEPT135 spectra (150 MHz) data for compound **5** in CH_3OH-d_4

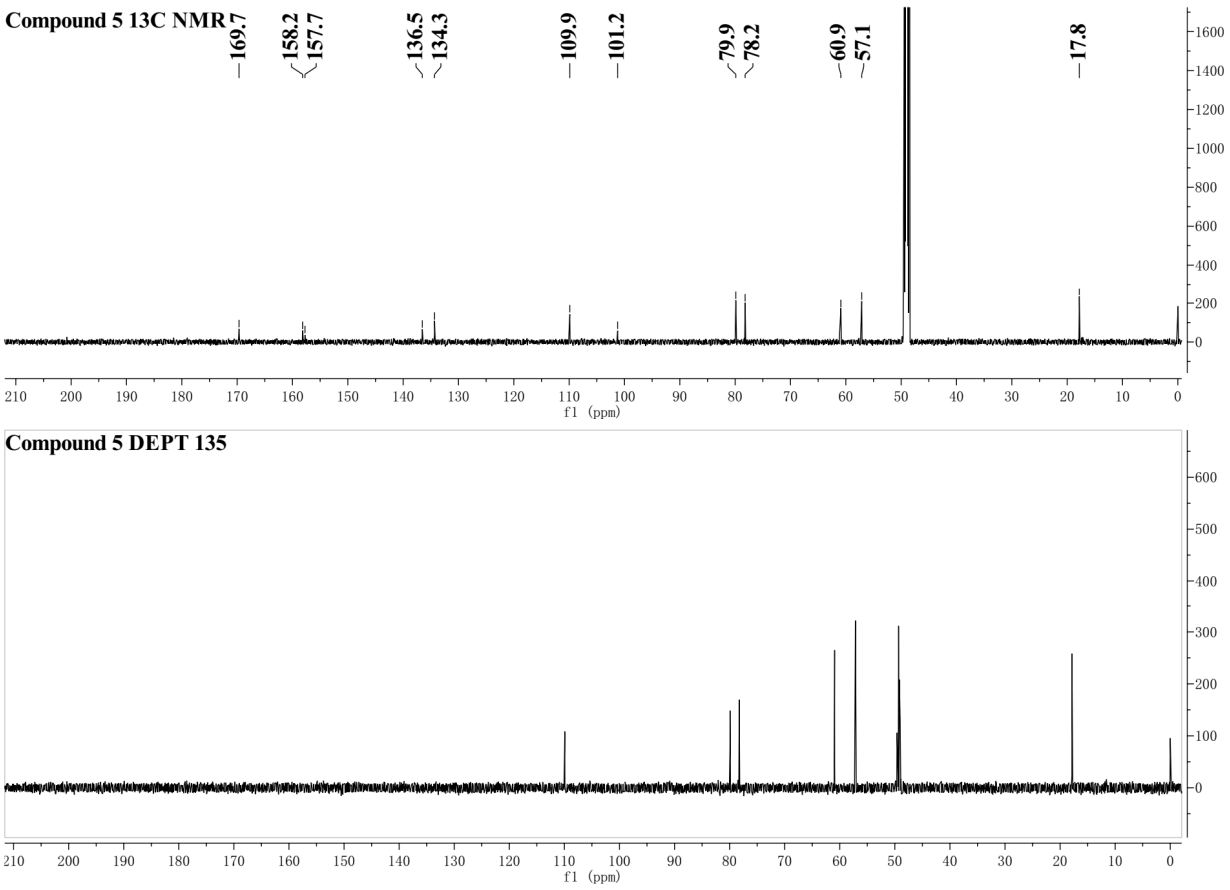


Figure S29. HSQC spectrum (600 MHz) of compound **5** in CH_3OH-d_4

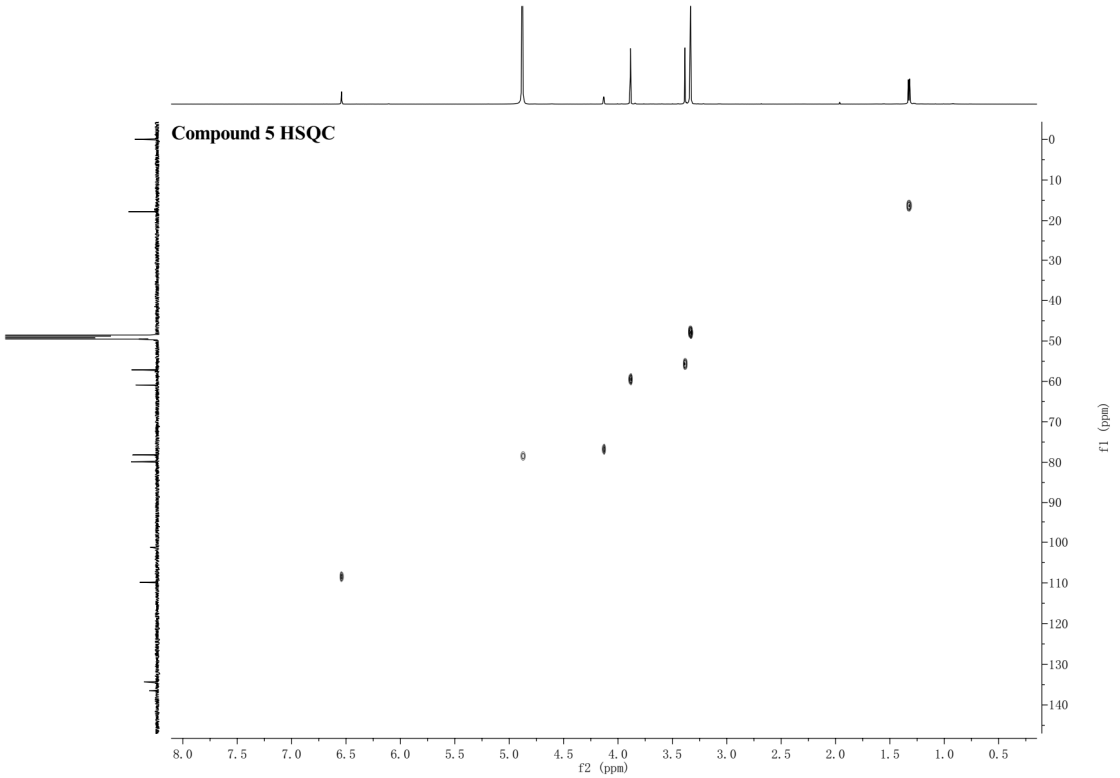


Figure S30. ^1H-^1H COSY spectrum (600 MHz) of compound **5** in CH_3OH-d_4

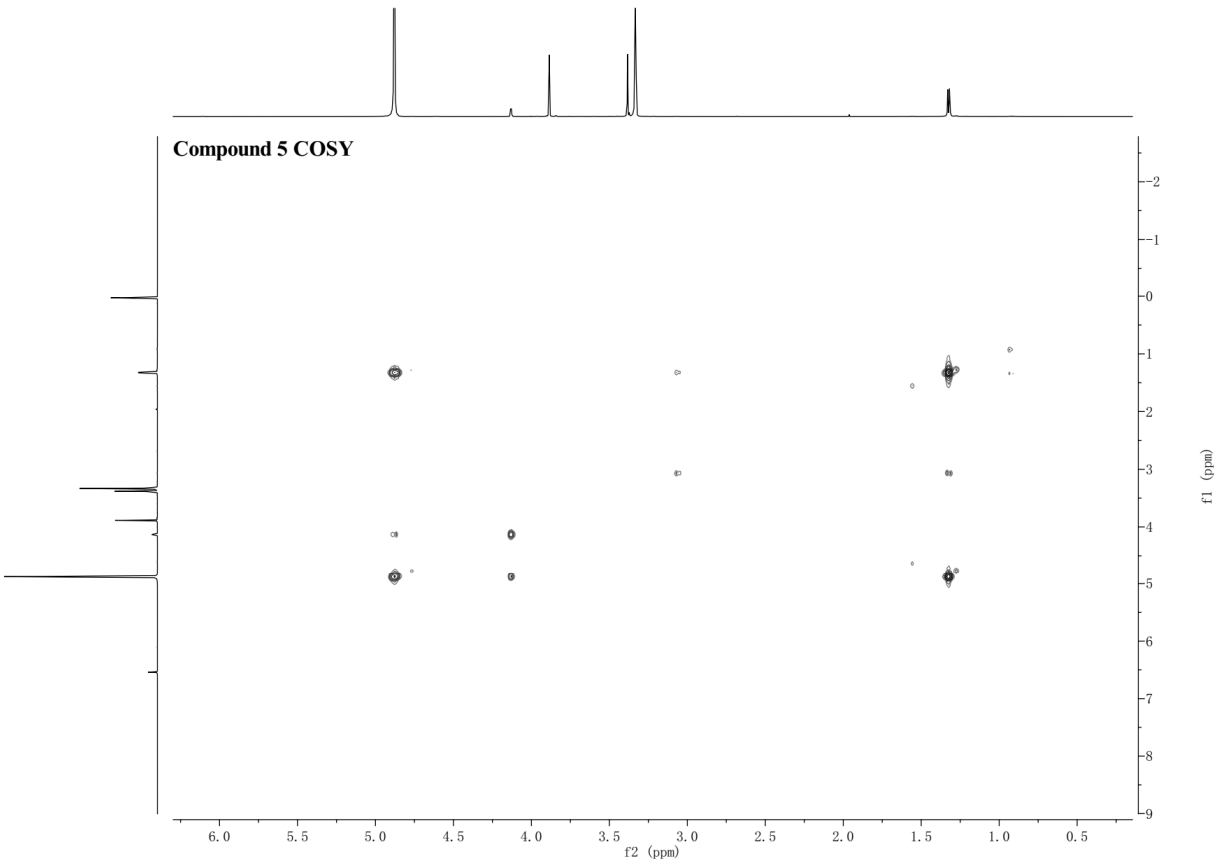


Figure S31. HMBC spectrum (600 MHz) of compound **5** in CH_3OH-d_4

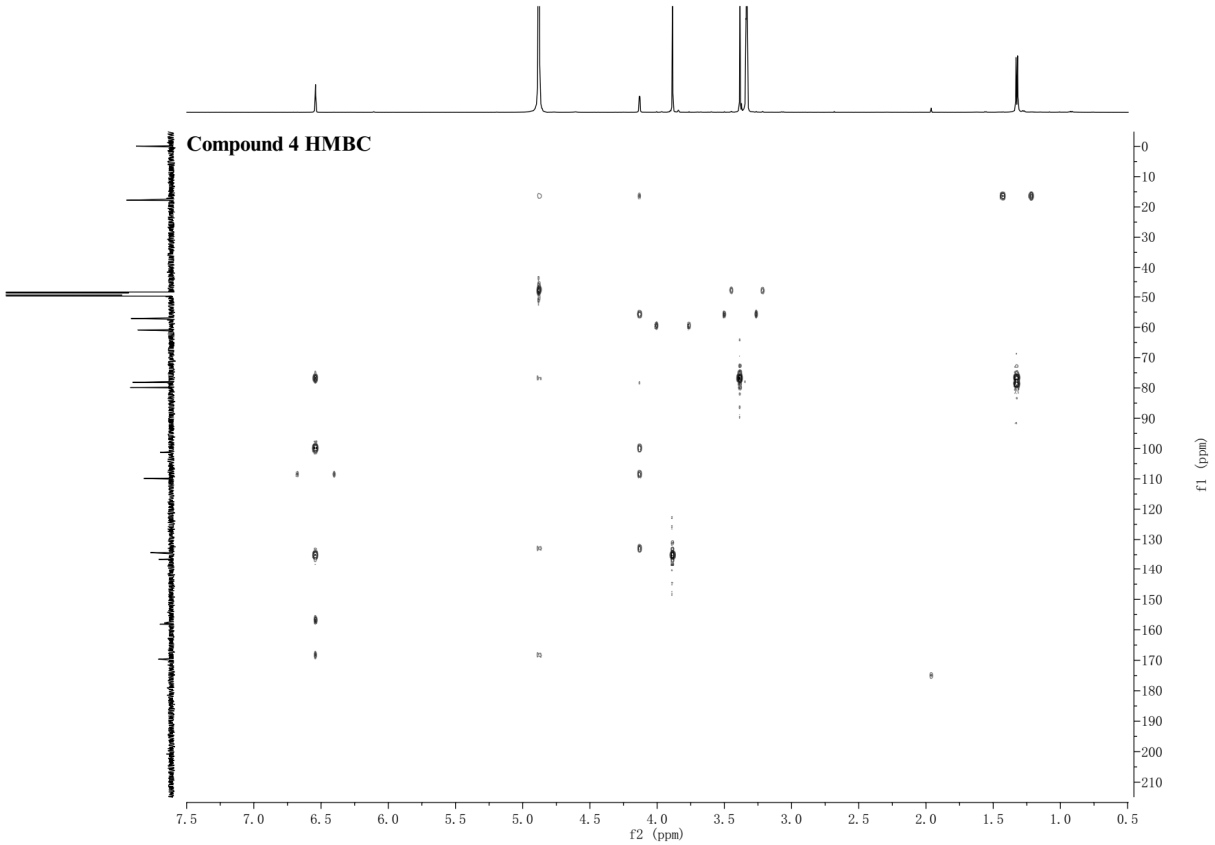


Figure S32. ROESY spectrum (500 MHz) of compound **5** in CH_3OH-d_4

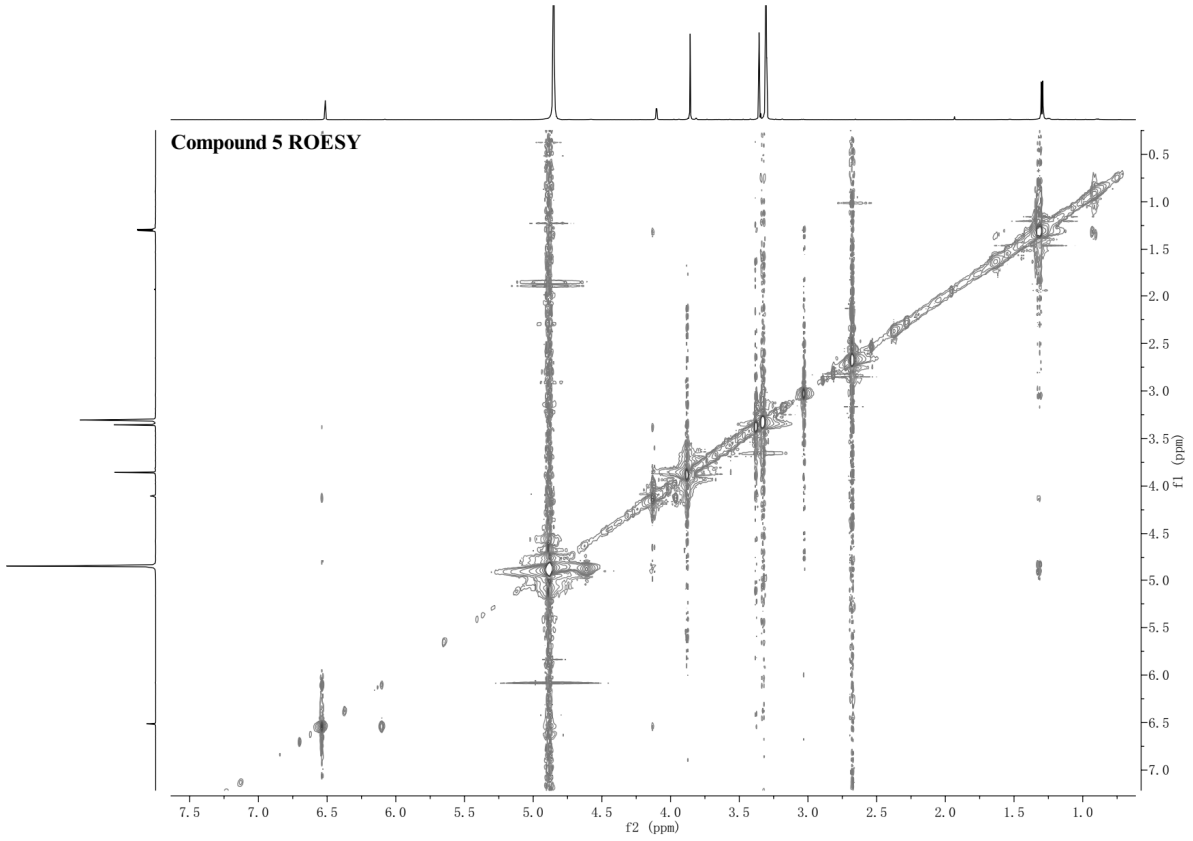


Figure S33. 1D NOESY spectrum (500 MHz) of compound **5** in CH_3OH-d_4

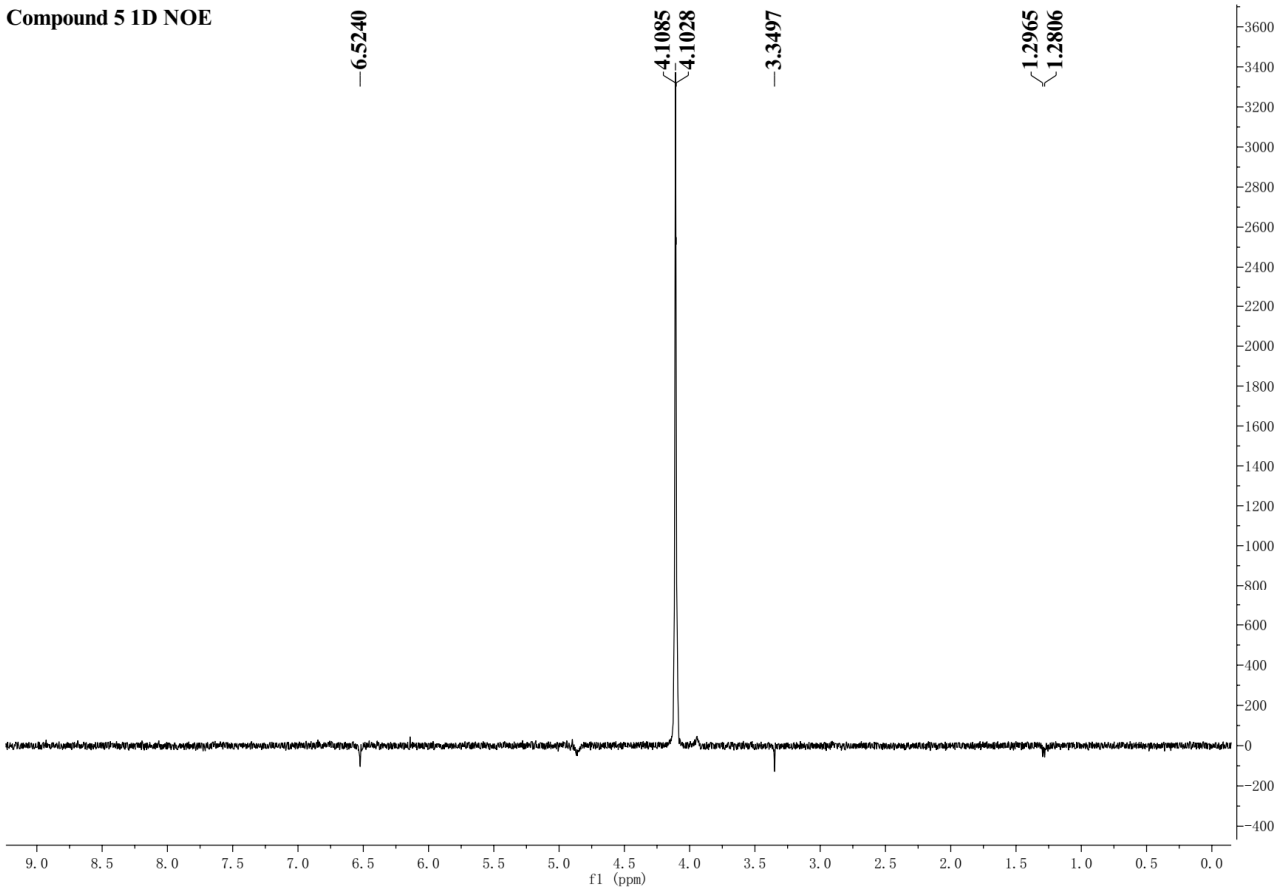
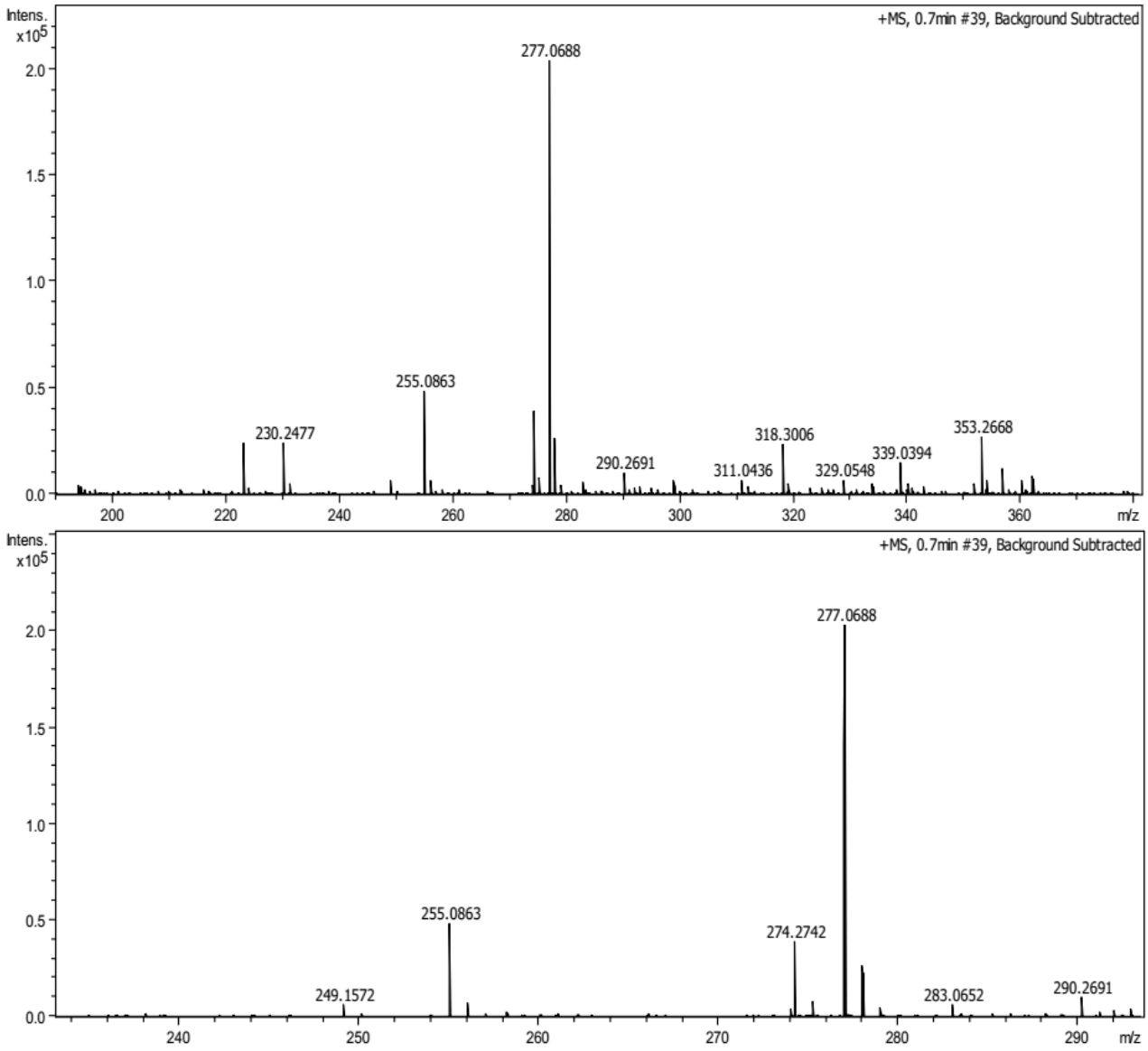


Figure S34. HRESIMS spectrum for compound **5**



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
255.08631		$C_{12}H_{15}O_6$	255.0863	-0.0	4.4	1	100.00	5.5	even	ok	$(M+H^+)$
277.06881		$C_{12}H_{14}NaO_6$	277.0683	-1.9	2.0	1	100.00	5.5	even	ok	$(M+Na^+)$

Table S1. ^{1}H and ^{13}C NMR Data for compound **6** and 6,8-dihydroxy-7-methoxy-3-methyl-isocoumarin in CH_3OH-d_4

Position	**6**		**6,8-dihydroxy-7-methoxy-3-methylisocoumarin**	
	δ_C, type	**δ_H mult. (*J* in Hz)**	**δ_C, type**	**δ_H mult. (*J* in Hz)**
1	168.1, C	—	168.2, C	—
2	—	—	—	—
3	154.6, C	—	154.6, C	—
4	105.3, CH	6.29, s	105.3, CH	6.30, s
5	103.7, CH	6.37, s	104.0, CH	6.38, s
6	160.0, C	—	161.0, C	—
7	135.2, C	—	135.5, C	—
8	156.1, C	—	156.2, C	—
9	100.4, C	—	100.0, C	—
10	136.1, C	—	136.2, C	—
11	19.1, CH_3	2.22, s	19.1, CH_3	2.19, s
12	61.0, CH_3	3.86, s	60.9, CH_3	3.84, s

Table S2. ^{1}H and ^{13}C NMR Data for compound **7** and Diaporthein A in $CHCl_3$-d

Position	**7**		**Diaporthein A**	
	δ_C, type	**δ_H mult. (*J* in Hz)**	**δ_C, type**	**δ_H mult. (*J* in Hz)**
1	24.8, CH_2	1.70, m; 1.82, m	24.8, CH_2	1.70, m; 1.82, m
2	18.0, CH_2	1.61, m; 1.67, m	18.0, CH_2	1.61,m; 1.67, m
3	37.7, CH_2	1.22, m; 1.69, m	37.8, CH_2	1.22, m; 1.69, m
4	38.0, C	—	38.0, C	—
5	81.3, C	—	81.3, C	—
6	105.9, C	—	105.9, C	—
7	73.3, CH	4.63, d, (2.2)	73.3, CH	4.63, d, (2.1)
8	136.8, C	—	136.8, C	—
9	77.1,C	—	77.1, C	—
10	50.1, C	—	50.1, C	—
11	67.3, CH	3.86, dd, (12.1, 4.2)	67.3, CH	3.86, dd, (12.0, 4.2)
12	40.4, CH_2	1.71, m; 1.89, m,	40.4, CH_2	1.71, m; 1.89, m
13	38.4, C	—	38.3, C	—
14	133.3, CH	5.99, dd, (1.6, 1.6)	133.3, CH	5.99, dd, (1.6, 1.7)
15	146.4, CH	5.85, dd, (17.5, 10.6)	146.4, CH	5.85, dd, (17.5, 10.7)
16	111.5, CH_2	5.04, m	111.5, CH_2	5.04, m
17	25.3, CH_3	1.16, s	25.3, CH_3	1.16, s
18	29.6, CH_3	1.25, s	29.6, CH_3	1.26, s
19	24.3, CH_3	1.43, s	24.2, CH_3	1.44, s
20	68.4, CH_2	3.35, d, (9.7); 3.97, d, (9.7)	68.3, CH_2	3.36, d, (9.6); 3.97, d, (9.6)

Table S3. ^{1}H and ^{13}C NMR Data for compound **8** and Diaporthein B in $CHCl_3$-*d*

Position	8		Diaporthein B	
	δ_C, type	δ_H mult. (*J* in Hz)	δ_C, type	δ_H mult. (*J* in Hz)
1	25.2, CH_2	1.96, m; 2.03, m	25.2, CH_2	1.96, m; 2.03, m
2	17.7, CH_2	1.62, m; 1.68, m	17.6, CH_2	1.62, m; 1.68, m
3	37.5, CH_2	1.24, m; 1.56, m	37.5, CH_2	1.23, m; 1.55, m
4	37.3, C	—	37.3, C	—
5	81.9, C	—	81.9, C	—
6	104.1, C	—	104.1, C	—
7	196.3, C	—	196.2, C	—
8	134.6, C	—	134.7, C	—
9	76.2,C	—	76.2, C	—
10	51.1, C	—	51.1, C	—
11	67.7, CH	4.04, dd, (11.7, 4.1)	67.7, CH	4.03, dd, (11.7, 4.1)
12	39.9 , CH_2	1.73, m; 2.07, m,	39.9, CH_2	1.73, m; 2.07, m
13	40.0, C	—	40.1, C	—
14	150.5, CH	6.82, d, (1.9)	150.4, CH	6.81, d, (1.8)
15	144.0, CH	5.83, dd, (17.5, 10.5)	144.1, CH	5.82, dd, (17.5, 10.7)
16	113.1, CH_2	5.09, d, m	113.1, CH_2	5.09, m
17	25.9, CH_3	1.22, s	25.9, CH_3	1.22, s
18	27.0, CH_3	1.20, s	26.9, CH_3	1.19, s
19	23.6, CH_3	1.44, s	23.7, CH_3	1.45, s
20	68.6, CH_2	3.72, d, (10.2); 4.14, d, (10.1)	68.6, CH_2	3.71, d, (10.2); 4.14, d, (10.2)